A Complete Bibliography of Publications in *Journal of Computational Chemistry*: 2010–2019

Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: beebe@math.utah.edu, beebe@acm.org, beebe@computer.org (Internet)
WWW URL: https://www.math.utah.edu/~beebe/

25 April 2024
Version 1.41

Title word cross-reference

[YZL^{+}15]. $[5+2]$ [LXFC17]. $[n]$ [uLhY11]. $^{+}$ [DDM^{+}15, FD16, FHG^{+}19, GMBM18, HDM^{+}19, LCL^{+}10, LdSRR16, LTR18, LCWW10, NH19, RLA^{+}11, RRF11, SS19, SFBT17, UT14, YCGA10, YZ15b, ZCK^{+}16, ZWY^{+}10a]. $^{+/0/-}$ [TG12b]. $^{+}\cdots\pi$ [CCCLCGRO14]. $^{-}$ [ATP18, CXW14, HBL12, JLH^{+}14, LCWW10, RDT14, TDT19, YCGA10, Yu12a, ZWY^{+}10b]. $^{-}_{18}$ [YLT^{+}19]. $^{0/+}$ [GTT10]. $^{0/+}$ [TN12]. ^{1} [Ben17, KSK11, LGW12, LX11, LWD13, PTK11, Pie14]. ^{11} [HJ13]. ^{129} [SKMS13]. ^{13} [Ben17, GMSV14, HJ13, OPR16, PTK11, Pie14, VAMS14]. ^{15} [RDT14]. $^{15}_{2}$ [RDT14]. ^{19} [DKE^{+}17]. $^{1}\Delta_g$ [WLF19]. $^{1}\Sigma$ [LWD13]. $^{1}\Sigma^{+}$ [Kop15b]. $^{1}\Sigma_g^{+}$ [ZZZ^{+}19]. ^{2} [GTK10, LGW12, LWD13, OZLSBH12]. $^{2+}$ [BHB^{+}17, BHB19, BMFG16, DAdGR15, LBC^{+}19, LPE^{+}10, LWXC16, MG11, PGY15, RRF11, RHT^{+}15, TLY^{+}12, WRG^{+}17, vSGP10]. $^{2-}_{18}$ [YLT^{+}19]. ^{29} [HAI^{+}16]. $^{2\bullet-}$ [LGW12]. $^{2}\Pi$ [GTK10, LWD13]. ^{3} [GTK10, HZ11, HCD^{+}10, TCPPC14, dCRN18]. $^{3+}$ [DAdGR15]. $^{3-}$ [RDT14]. ^{31} [HAI^{+}16]. ^{35} [Tsi19]. $^{4+}$ [YW12]. ^{43} [HBI^{+}17]. ^{51} [MG11]. ^{77} [RK15]. ^{I} [WJX^{+}10]. ^{II} [CM16]. ^{IV} [LLSW14, MG11]. ^{LHM} [BS10c]. ^{p} [vSGP10]. $'$ [KPL15]. $_{(ads)}$ [LLTC12]. $_{1}$ [ILKR11, II10, KIOY19]. $_{1}+x$ [SMiN^{+}19]. $_{1,2}$ [WHL^{+}10]. $_{10}$ [GSS13, LdSRR16, TFQ^{+}11, WWKS16]. $_{1}2$ [BHP19, CC18c, DM15, LLLM11, LLB^{+}12, LLD17, LCWW10, VIT^{+}15]. $_{13}$ [JCG^{+}11, LAHS16, SC17]. $^{+}_{13}$ [OPR16]. $^{+}_{15}$ [OPR16]. $_{16}$ [WZH^{+}18]. $_{18}$ [DM15, TFQ^{+}10, VIT^{+}15]. $_{19}$ [DM15, VIT^{+}15]. $^{-}_{19}$ [YLZ^{+}19]. $_{2}$ [AS15a, AR10, BE14, BPE16, BŁF14, BCNH^{+}11, BPLL12, BLG10, BWKW10a, BWKW10b, BS10b, BS16b, CK10, CCJ^{+}11, CCM15, CKL^{+}11, CXS10, CSNCS^{+}18, DSB^{+}19, DOM^{+}11, DLSD13, DT19, DLW12, DHE^{+}12, DSHLM18, EVR18, EP15, EBPK17b, EB18, FMNC11, GLZ17, GK10, GWJR18, GNI18, GY12, GWJJ12, HSJ18, HYL^{+}11, HZ11, HSY^{+}11, HFSO12, HBL12, HYD10, HRL11, HVS16, Ibr17, JCG^{+}10, JLS^{+}10, JLH^{+}14, KBC12, KIOY19, KMS^{+}19, KKR^{+}13, Kop16, Kop18, Kop19b, KCL^{+}14, LZTV10, LWW12, LYC^{+}13, LAHS16, LBTV12, LLSW14, LWXC16, LLLW19, LPLB16, LCWW10, LWD13, LJG^{+}11, LLL^{+}12, MLQ^{+}12, MLGB16, MP19a, MG15, MKH15, MCUJ15, MLCD11, MS15, MCAY15, NGAS17, NC14, NMLD13, NKD18, OKY18, PVL^{+}13, PLFS18, PBE16, RHNN10, RAGLL11, RDT14, RRC^{+}15, RVdMB16, RHT^{+}15, RSKG14, RSK^{+}15, SSC^{+}19, ŠBD^{+}17, SC17, STS^{+}10]. $_{2}$ [SSX^{+}14, SLY^{+}19, TLdG^{+}12, TNY18, Tak11, TSJ^{+}10, TSZQ12, Tsi17, UvSvdWK19, VP19, VT14, VV14, WKC10a, WHL^{+}10, WGL^{+}11, WMW11, WLHZ12, WC13, WWKS16, WLF19, WRM^{+}12, WGN^{+}16, WGLG^{+}16, WYGW12, XFX^{+}16, XCLZ19, YR13, YHX19, YLL11, Yu12a, YZ15b, YXZZ17, ZRCC11, ZRCC12, ZZ10, ZZL^{+}10b, ZSWL12, ZLLL12, ZYG^{+}14, ZLY^{+}16, ZZZ^{+}19, ZZL19, dSDdAR10]. $_{20}$ [GBGR16, JCG^{+}11, LdSRR16, MCK17b]. $^{-}_{20}$ [YLZ^{+}19]. $_{24}$ [GBGR16, YW12]. $_{26}$ [LAHS16]. $_{28}$ [MCK17a]. $^{+}_{2}$ [CG12, EVR18, MH11]. $^{-}_{2}$ [MN19, Sak18]. $_{2h}$ [ZLY^{+}16]. $_{3}$ [Alg17, AR10, ATP18, ASS^{+}17, ABB^{+}12, ABB^{+}13, BE12, CK10, CCJ^{+}11, CXW14, EB12, EBK13, FD16, FHG^{+}19, GSMZ19, HSJ18, HDM^{+}19, Ibr17, JCG^{+}10, KT19, KKR^{+}13, LLBO12, LLLM11, LLB^{+}12,

Ano14-42, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-50, Ano14-51, Ano14-52, Ano14-53, Ano14-54, Ano14-55, Ano14-27, Ano14-48, Ano14-49, Ano14-56, Ano14-57, Ano14-58, Ano14-59, Ano14-60, Ano14-61, Ano14-62, Ano14-63, Ano14-64, Ano14-65, Ano14-66, Ano14-67, Ano14-68, Ano14-69, Ano14-70, Ano14-71, Ano14-72, Ano14d, Ano14e, Ano14f, Ano15a, Ano15b, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o]. **Issue** [Ano15p, Ano15q, Ano15r, Ano15s, Ano15t, Ano15u, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15-35, Ano15-36, Ano15-39, Ano15v, Ano15-40, Ano15-41, Ano15-42, Ano15-43, Ano15-44, Ano15w, Ano15x, Ano15-37, Ano15-38, Ano15-45, Ano15-46, Ano15-47, Ano15-48, Ano15-49, Ano15-50, Ano15-51, Ano15-52, Ano15-53, Ano15-54, Ano15-55, Ano15-56, Ano15-57, Ano15c, Ano15d, Ano15e, Ano15f, Ano15g, Ano15h, Ano16a, Ano16b, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m, Ano16n, Ano16o, Ano16p, Ano16q, Ano16r, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16-29, Ano16-30, Ano16-31, Ano16-32, Ano16-33, Ano16-34, Ano16-35, Ano16-36, Ano16c, Ano16-39, Ano16-40, Ano16-41, Ano16s, Ano16t]. **Issue** [Ano16-37, Ano16-38, Ano16-42, Ano16-43, Ano16-44, Ano16-45, Ano16-46, Ano16-47, Ano16-48, Ano16-49, Ano16-50, Ano16-51, Ano16-52, Ano16-53, Ano16-54, Ano16-55, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16-75, Ano16-89, Ano16-80, Ano16-94, Ano16-81, Ano16-95, Ano16-82, Ano16-96, Ano16-83, Ano16-97, Ano16-84, Ano16-98, Ano16-85, Ano16-99, Ano16-86, Ano16-100, Ano16-87, Ano16-101, Ano16-88, Ano16-102, Ano16-76, Ano16-90, Ano16-77, Ano16-91, Ano16-78, Ano16-92, Ano16-79, Ano16-93, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130, Ano16-111, Ano16-112, Ano16-113, Ano16-114, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Ano16-115, Ano16-121, Ano16-122, Ano16-123, Ano16-124, Ano16-125, Ano16-126, Ano16-127, Ano16-128, Ano16-116, Ano16-117, Ano16-118, Ano16-119, Ano16-120, Ano16-57, Ano16-58, Ano16-59, Ano16-60, Ano16-61, Ano16-62, Ano16-63]. **Issue** [Ano16-64, Ano16-65, Ano16-66, Ano16-67, Ano16-68, Ano16-69, Ano16-70, Ano16-71, Ano16-72, Ano16-73, Ano16-74, Ano17a, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17z, Ano17-27, Ano17-28, Ano17y, Ano17-29, Ano17-30, Ano17-31, Ano17-32, Ano17-33, Ano17-34, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17l, Ano17m, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano17-36, Ano17-37, Ano17-62, Ano17-63, Ano17-64, Ano17-65, Ano17-66, Ano17-67, Ano17-38, Ano17-39, Ano17-40, Ano17-41, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano17-51, Ano17-52, Ano17-53, Ano17-54, Ano17-55, Ano17-56, Ano17-57, Ano17-58, Ano17-59, Ano17-60, Ano17-61, Ano18a, Ano18b, Ano18t, Ano18u, Ano18v, Ano18w, Ano18x, Ano18y]. **Issue** [Ano18z, Ano18-27, Ano18-28, Ano18-30, Ano18-31, Ano18-32, Ano18n, Ano18-29, Ano18-33, Ano18-34, Ano18-35, Ano18-36, Ano18-37, Ano18-38, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18h, Ano18i, Ano18j, Ano18k,

[MM19, KNR$^+$18]. **resolving** [AVHB18]. **resonance** [EFS16, GWW19, KNP$^+$12, PLFS18, Ran19, YB13]. **resource** [Gil11]. **respiratory** [TNI19b]. **Response** [GPGSM12, dSdS12b, BZH14, DSAS19, DHE$^+$12, ESM$^+$12, ITIN15, KSSH13, Kid19, KZK$^+$12, LP11b, MRB14, RJR14, RCM$^+$13b, SS16a, SDF$^+$17, WGLG$^+$16]. **responses** [GWX$^+$12, MLQ$^+$12]. **responsive** [MBA14]. **restrained** [ER18, HCD$^+$10, KCK$^+$17, SR18, ZDZM13]. **restraining** [KOY$^+$12]. **restraint** [RO14a]. **restraints** [LL19b, SM11]. **Restricted** [SL10, Cas13, PDG$^+$16, YD17]. **restriction** [FSD$^+$18]. **result** [PH15]. **resulting** [MvBD18]. **Results** [XKW18, Ber17, CBH14, CLK11, GR10a, KERY$^+$16, PŁAG11, RAR$^+$11, SHL$^+$13, SPZP18b, WDHZ13, KMLS10]. **retinal** [CG12, GA18, SGWA17, WGA18, ZLHH14]. **retinoic** [LFM12]. **Retracted** [Ano12u, GRL$^+$12]. **retro** [GRCL12]. **retro-imino-ene** [GRCL12]. **reveal** [MA16, RKDM14]. **revealed** [ALH$^+$10, KKK$^+$19, PNG10, VKNT15, YZGS14b, YJ19]. **Revealing** [VVY17, YW13, YJ17, Bac12, GFGS18]. **reveals** [NR11, WC11]. **Reverse** [KZP$^+$18b, LWL$^+$16, LLH$^+$19, ASL$^+$11, Aou16, GP12, OPBR17]. **reversible** [RIJ$^+$11]. **Review** [CD19, DR14, FRSA14, GHV17, JCL$^+$17, LJC$^+$19, CMvG10, Sch10, Spr10]. **Reviews** [HLvdV13, ZZWT12]. **Revised** [AKMYB18, CKG18]. **Revising** [Pla11]. **Revision** [PLH16]. **Revisit** [WZH$^+$18]. **Revisited** [KR14, ASS$^+$17, CYI$^+$10, Dil15, HZ11, HFSO12, MSBF16, YW13, vSGP10]. **Revisiting** [OAN15a, Sán17, dSVdM$^+$16]. **Revitalizing** [SZL19]. **reweighted** [SH11b]. **reweighting** [Fer17, OGL10]. **Rh** [KSO$^+$19, SN16a, WJX$^+$10]. **Rh-catalyzed** [KSO$^+$19]. **rhenium** [TS15a, ZWMW10]. **Rhodium** [BF19b, GYX$^+$10, RLD12]. **rhodopsin** [RLG11]. **rhodopsins** [HRMAL$^+$13]. **rhombohedral** [BE12]. **Rhorix** [MSSP17]. **rhOver** [BP18]. **RI** [BK17c, BK17c, ISM18, KNHN16, TKN13, RKGN10]. **RI-MP2** [BK17c, KNHN16, TKN13, RKGN10]. **RI-MP3** [ISM18]. **ribonucleotides** [XVA$^+$16]. **ribozyme** [BJSI12]. **ribulose** [CKG18]. **ribulose-1** [CKG18]. **rich** [BHI19, ZZWX11, ZYL$^+$12, YZWC11]. **right** [SJWE10]. **Rigid** [NJR18, Aou16, AGR11a, CZNA11, DBM$^+$17, HDL$^+$14, ODB18, PG14, PGK$^+$19, dACP12]. **rigid-body** [PGK$^+$19]. **Rigid-CLL** [dACP12]. **Rigidity** [NPG17, OXBW16, PRSG13]. **rigorous** [WO15]. **ring** [ABDGN12, CPN$^+$17, CB11d, FNSF$^+$11, GWT$^+$17, GMBX$^+$16, GSMZ19, HH10, HH11, HCD$^+$10, LGC19, PCLL11, PLH16, SP13, WCL$^+$11, XVN17, YHCS11, ZQ14, OSI$^+$19]. **ring-closure** [ABDGN12]. **ring-conformational** [PLH16]. **ring-opening** [GMBX$^+$16, GSMZ19, LGC19, WCL$^+$11, ZQ14]. **ring-polycyclic** [CB11d]. **rings** [FNSF$^+$11, GLF16, JHH$^+$13, PRJ$^+$17, Ran19, TDKT10, ZSTRS$^+$18]. **RISM** [HNN$^+$17, MYT$^+$14]. **RM1** [VSA11]. **RM1-based** [VSA11]. **RMC_POT** [GP12]. **RMSD** [CW19]. **RMSDs** [PG14]. **RNA** [Clo15, DPNM11, GTZ$^+$18, HZ13, KT10, LM18a, SM11, WXY14, XHLH16]. **RNA-binding** [XHLH16]. **roaming** [CSNCS$^+$18]. **robust**

References

Anderson:2018:GSZ

[AA18] James S. M. Anderson and Paul W. Ayers. The general setting for the zero-flux condition: the Lagrangian and zero-flux conditions that give the Heisenberg equation of motion. *Journal of Computational Chemistry*, 39(17):1051–1058, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andres:2019:NQE

[AAB+19] Juan Andrés, Paul W. Ayers, Roberto A. Boto, Ramon Carbó-Dorca, Henry Chermette, Jerzy Cioslowski, Julia Contreras-García, David L. Cooper, Gernot Frenking, Carlo Gatti, Farnaz Heidar-Zadeh, Laurent Joubert, Ángel Martín Pendás, Eduard Matito, István Mayer, Alston J. Misquitta, Yirong Mo, Julien Pilmé, Paul L. A. Popelier, Martin Rahm, Eloy Ramos-Cordoba, Pedro Salvador, W. H. Eugen Schwarz, Shant Shahbazian, Bernard Silvi, Miquel Solà, Krzysztof Szalewicz, Vincent Tognetti, Frank Weinhold, and Émilie-Laure Zins. Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, 40(26):2248–2283, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aquilante:2016:SNU

[AAC+16] Francesco Aquilante, Jochen Autschbach, Rebecca K. Carlson, Liviu F. Chibotaru, Mickaël G. Delcey, Luca De Vico, Ignacio Fdez. Galván, Nicolas Ferré, Luis Manuel Frutos, Laura Gagliardi, Marco Garavelli, Angelo Giussani, Chad E. Hoyer, Giovanni Li Manni, Hans Lischka, Dongxia Ma, Per Åke Malmqvist, Thomas Müller, Artur Nenov, Massimo Olivucci, Thomas Bondo Pedersen, Daoling Peng, Felix Plasser, Ben Pritchard, Markus Reiher, Ivan Rivalta, Igor Schapiro, Javier

Segarra-Martí, Michael Stenrup, Donald G. Truhlar, Liviu Ungur, Alessio Valentini, Steven Vancoillie, Valera Veryazov, Victor P. Vysotskiy, Oliver Weingart, Felipe Zapata, and Roland Lindh. Software news and updates: Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, 37(5):506–541, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abdel-Azeim:2011:ZHB

[AALCM11] Safwat Abdel-Azeim, Xin Li, Lung Wa Chung, and Keiji Morokuma. Zinc–homocysteine binding in cobalamin-dependent methionine synthase and its role in the substrate activation: DFT, ONIOM, and QM/MM molecular dynamics studies. *Journal of Computational Chemistry*, 32(15):3154–3167, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Altarawneh:2011:RCH

[AAMD+11] Mohammednoor Altarawneh, Ala'A H. Al-Muhtaseb, Bogdan Z. Dlugogorski, Eric M. Kennedy, and John C. Mackie. Rate constants for hydrogen abstraction reactions by the hydroperoxyl radical from methanol, ethenol, acetaldehyde, toluene, and phenol. *Journal of Computational Chemistry*, 32 (8):1725–1733, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akbarzadeh:2018:PCN

[AAMR18] Hamed Akbarzadeh, Mohsen Abbaspour, Esmat Mehrjouei, and Samira Ramezanzadeh. Pt-Co nanocluster in hollow carbon nanospheres. *Journal of Computational Chemistry*, 39 (19):1267–1274, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Achazi:2017:CSS

[AARP17] Andreas J. Achazi, Dirk Andrae, Hans-Ulrich Reissig, and Beate Paulus. A computational study of samarium diiodide-induced cyclizations of *N*-oxoalkyl-substituted methyl indole-3-carboxylates — a rationale of the diastereoselectivity. *Journal of Computational Chemistry*, 38(31):2693–2700, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abbaspour:2018:MDS

[AASP18] Mohsen Abbaspour, Hamed Akbarzadeh, Sirous Salemi, and Khodanazar Pirfalak. Molecular dynamics simulation of liquid water and ice nanoclusters using a new effective HFD-like model. *Journal of Computational Chemistry*, 39(5):269–278, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abolfath:2010:DBR

[AB10] Ramin M. Abolfath and Thomas Brabec. DNA-backbone radio resistivity induced by spin blockade effect. *Journal of Computational Chemistry*, 31(14):2601–2606, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arthur:2016:EIC

[AB16a] Evan J. Arthur and Charles L. Brooks III. Efficient implementation of constant pH molecular dynamics on modern graphics processors. *Journal of Computational Chemistry*, 37(24): 2171–2180, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arthur:2016:PIG

[AB16b] Evan J. Arthur and Charles L. Brooks III. Parallelization and improvements of the generalized born model with a simple switching function for modern graphics processors. *Journal of Computational Chemistry*, 37(10):927–939, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Antoniotti:2012:GPR

[ABB+12] Paola Antoniotti, Elena Bottizzo, Stefano Borocci, Maria Giordani, and Felice Grandinetti. Gas-phase reactions of SiH_n^+ ($n = 1, 2$) with NF_3: a computational investigation on the detailed mechanistic aspects. *Journal of Computational Chemistry*, 33(24):1918–1926, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [ABB+13].

Antoniotti:2013:EGP

[ABB+13] Paola Antoniotti, Elena Bottizzo, Stefano Borocci, Maria Giordani, and Felice Grandinetti. Erratum: Gas-phase reactions of SiH_n^+ ($n = 1, 2$) with NF_3: a computational investigation on the detailed mechanistic aspects [J. Comp. Chem. **33**, 1918–1926]. *Journal of Computational Chemistry*, 34(3): 257, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [ABB+12].

Alakent:2011:ELB

[ABD11] Burak Alakent, Sena Baskan, and Pemra Doruker. Effect of ligand binding on the intraminimum dynamics of proteins. *Journal of Computational Chemistry*, 32(3):483–496, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andres:2012:NRC

[ABDGN12] J. Andrés, S. Berski, L. R. Domingo, and P. González-Navarrete. Nature of the ring-closure process along the rearrangement of octa-1,3,5,7-tetraene to cycloocta-1,3,5-triene from the perspective of the electron localization function and catastrophe theory. *Journal of Computational Chemistry*, 33 (7):748–756, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allen:2015:DIN

[ABM+15] William J. Allen, Trent E. Balius, Sudipto Mukherjee, Scott R. Brozell, Demetri T. Moustakas, P. Therese Lang, David A. Case, Irwin D. Kuntz, and Robert C. Rizzo. DOCK 6: Impact of new features and current docking performance. *Journal of Computational Chemistry*, 36(15):1132–1156, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:2011:PEG

[Abr11] Mark J. Abraham. Performance enhancements for GROMACS nonbonded interactions on BlueGene. *Journal of Computational Chemistry*, 32(9):2041–2046, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arrar:2019:AEF

[ABS+19] Mehrnoosh Arrar, Fernando Martín Boubeta, Maria Eugenia Szretter, Mariela Sued, Leonardo Boechi, and Daniela Rodriguez. On the accurate estimation of free energies using the Jarzynski equality. *Journal of Computational Chemistry*, 40(4):688–696, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anisimov:2011:QMB

[AC11a] Victor M. Anisimov and Claudio N. Cavasotto. Quantum mechanical binding free energy calculation for phosphopeptide inhibitors of the Lck SH2 domain. *Journal of Computational Chemistry*, 32(10):2254–2263, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Avaltroni:2011:ERS

[AC11b] Fabrice Avaltroni and Clemence Corminboeuf. Efficiency of random search procedures along the silicon cluster series: Si_n (n = 5–10, 15, and 20). *Journal of Computational Chemistry*, 32(9):1869–1875, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Avaltroni:2012:ICL

[AC12] Fabrice Avaltroni and Clemence Corminboeuf. Identifying clusters as low-lying minima — efficiency of stochastic and genetic algorithms using inexpensive electronic structure levels. *Journal of Computational Chemistry*, 33(5):502–508, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Adhikari:2013:EST

[ACD+13a] Kalipada Adhikari, Sudip Chattopadhyay, Barin Kumar De, Amitava Sharma, Ranendu Kumar Nath, and Dhiman Sinha. Erratum: Search of truncation of $(N-1)$ electron basis containing full connected triple excitations in computing main and satellite ionization potentials via Fock space coupled cluster approach. *Journal of Computational Chemistry*, 34(24): 2133, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [ACD+13b].

Adhikari:2013:STE

[ACD+13b] Kalipada Adhikari, Sudip Chattopadhyay, Barin Kumar De, Amitava Sharma, Ranendu Kumar Nath, and Dhiman Sinha. Search of truncation of $(N-1)$ electron basis containing full connected triple excitations in computing main and satellite ionization potentials via Fock-space coupled cluster approach. *Journal of Computational Chemistry*, 34(15):1291–1310, June

5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [ACD+13a].

Asaduzzaman:2012:RBD

[ACS12] Abu Md. Asaduzzaman, Guy A. G. Chappellaz, and Georg Schreckenbach. Relationship between dye–iodine binding and cell voltage in dye-sensitized solar cells: a quantum-mechanical look. *Journal of Computational Chemistry*, 33 (31):2492–2497, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Affentranger:2010:PFC

[AD10] Roman Affentranger and Xavier Daura. Polypeptide folding on a conformational-space network: Dependence of network topology on the structural discretization procedure. *Journal of Computational Chemistry*, 31(9):1889–1903, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aquilante:2010:MNG

[ADF+10] Francesco Aquilante, Luca De Vico, Nicolas Ferré, Giovanni Ghigo, Per åke Malmqvist, Pavel Neogrády, Thomas Bondo Pedersen, Michal Pitoňák, Markus Reiher, Björn O. Roos, Luis Serrano-Andrés, Miroslav Urban, Valera Veryazov, and Roland Lindh. MOLCAS 7: the next generation. *Journal of Computational Chemistry*, 31(1):224–247, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anacker:2014:NAB

[AF14] Tony Anacker and Joachim Friedrich. New accurate benchmark energies for large water clusters: DFT is better than expected. *Journal of Computational Chemistry*, 35(8):634–643, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allen:2017:CND

[AFBR17] William J. Allen, Brian C. Fochtman, Trent E. Balius, and Robert C. Rizzo. Customizable de novo design strategies for DOCK: Application to HIVgp41 and other therapeutic targets. *Journal of Computational Chemistry*, 38(30):2641–2663, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Addicoat:2013:SSD

[AFPI13] Matthew A. Addicoat, Syou Fukuoka, Alister J. Page, and Stephan Irle. Stochastic structure determination for conformationally flexible heterogeneous molecular clusters: Application to ionic liquids. *Journal of Computational Chemistry*, 34(30):2591–2600, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anand:2016:HBA

[AFSW16] Megha Anand, Israel Fernández, Henry F. Schaefer III, and Judy I-Chia Wu. Hydrogen bond–aromaticity cooperativity in self-assembling 4-pyridone chains. *Journal of Computational Chemistry*, 37(1):59–63, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abraham:2011:OPM

[AG11] Mark J. Abraham and Jill E. Gready. Optimization of parameters for molecular dynamics simulation using smooth particle-mesh Ewald in GROMACS 4.5. *Journal of Computational Chemistry*, 32(9):2031–2040, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Antony:2012:FIP

[AG12] Jens Antony and Stefan Grimme. Fully ab initio protein-ligand interaction energies with dispersion corrected density functional theory. *Journal of Computational Chemistry*, 33(21):1730–1739, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anthopoulos:2013:GAM

[AGB13] Athanasios Anthopoulos, Ian Grimstead, and Andrea Brancale. GPU-accelerated molecular mechanics computations. *Journal of Computational Chemistry*, 34(26):2249–2260, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Astray:2013:EFP

[AGM+13] Gonzalo Astray, Juan F. Gálvez, Juan C. Mejuto, Oscar A. Moldes, and Iago Montoya. Esters flash point prediction using artificial neural networks. *Journal of Computational Chemistry*, 34(5):355–359, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Artemova:2011:CNS

[AGR11a] Svetlana Artemova, Sergei Grudinin, and Stephane Redon. A comparison of neighbor search algorithms for large rigid molecules. *Journal of Computational Chemistry*, 32(13):2865–2877, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Artemova:2011:FCA

[AGR11b] Svetlana Artemova, Sergei Grudinin, and Stephane Redon. Fast construction of assembly trees for molecular graphs. *Journal of Computational Chemistry*, 32(8):1589–1598, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alonso:2010:USA

[AH10] Mercedes Alonso and Bernardo Herradón. A universal scale of aromaticity for π-organic compounds. *Journal of Computational Chemistry*, 31(5):917–928, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ato:2019:TSC

[AHK$^+$19] Yoshinori Ato, Akihide Hayashi, Hiroaki Koga, Kohei Tada, Takashi Kawakami, Shusuke Yamanaka, and Mitsutaka Okumura. Theoretical study of correlations between the coordination structures and catalytic activities in polymer-stabilized au nanocluster catalysts. *Journal of Computational Chemistry*, 40(1):222–228, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Afanasyeva:2015:SNU

[AIGP15] Arina Afanasyeva, Sergey Izmailov, Michel Grigoriev, and Michael Petukhov. Software news and updates: AquaBridge: a novel method for systematic search of structural water molecules within the protein active sites. *Journal of Computational Chemistry*, 36(26):1973–1977, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Araki:2018:IAP

[AIM$^+$18] Mitsugu Araki, Hiroaki Iwata, Biao Ma, Atsuto Fujita, Kei Terayama, Yukari Sagae, Fumie Ono, Koji Tsuda, Narutoshi Kamiya, and Yasushi Okuno. Improving the Accuracy of

Protein-Ligand Binding Mode Prediction Using a Molecular Dynamics-Based Pocket Generation Approach. *Journal of Computational Chemistry*, 39(32):2679–2689, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abbaspour:2019:MDS

[AJA+19] Mohsen Abbaspour, Majid Namayandeh Jorabchi, Hamed Akbarzadeh, Sirous Salemi, and Reyhaneh Ebrahimi. Molecular dynamics simulation of anticancer drug delivery from carbon nanotube using metal nanowires. *Journal of Computational Chemistry*, 40(25):2179–2190, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Artemova:2016:AMS

[AJR16] Svetlana Artemova, Léonard Jaillet, and Stephane Redon. Automatic molecular structure perception for the universal force field. *Journal of Computational Chemistry*, 37(13):1191–1205, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aono:2010:PTP

[AK10] Shinji Aono and Shigeki Kato. Proton transfer in phenol–amine complexes: Phenol electronic effects on free energy profile in solution. *Journal of Computational Chemistry*, 31(16):2924–2931, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akimov:2016:SNU

[Aki16] Alexey V. Akimov. Software news and updates: Libra: an open-source “methodology discovery” library for quantum and classical dynamics simulations. *Journal of Computational Chemistry*, 37(17):1626–1649, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alekseenko:2016:SGI

[AKK+16] Andrey Alekseenko, Olga Kononova, Yaroslav Kholodov, Kenneth A. Marx, and Valeri Barsegov. SOP-GPU: influence of solvent-induced hydrodynamic interactions on dynamic structural transitions in protein assemblies. *Journal of Computational Chemistry*, 37(17):1537–1551, June 30, 2016.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abdula:2011:DND

[AKMT11] Ahmed Mutanabbi Abdula, Reema Abu Khalaf, Mohammad S. Mubarak, and Mutasem O. Taha. Discovery of new β- D-galactosidase inhibitors via pharmacophore modeling and QSAR analysis followed by in silico screening. *Journal of Computational Chemistry*, 32(3):463–482, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Adam:2018:RCF

[AKMYB18] Suliman Adam, Michaela Knapp-Mohammady, Jun Yi, and Ana-Nicoleta Bondar. Revised CHARMM force field parameters for iron-containing cofactors of photosystem II. *Journal of Computational Chemistry*, 39(1):7–20, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Awasthi:2016:SFE

[AKN16] Shalini Awasthi, Venkat Kapil, and Nisanth N. Nair. Sampling free energy surfaces as slices by combining umbrella sampling and metadynamics. *Journal of Computational Chemistry*, 37(16):1413–1424, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aleksandrov:2019:MMM

[Ale19] Alexey Aleksandrov. A molecular mechanics model for flavins. *Journal of Computational Chemistry*, 40(32):2834–2842, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Algarra:2017:CIT

[Alg17] Andrés G. Algarra. Computational insights into the S_3 transfer reaction: a special case of double group transfer reaction featuring bicyclically delocalized aromatic transition state geometries. *Journal of Computational Chemistry*, 38(22):1966–1973, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Azam:2010:HGI

[ALH+10] S. Sikander Azam, Len Herald V. Lim, Thomas S. Hofer, Bernhard R. Randolf, and Bernd M. Rode. Hydrated germanium (II): Irregular structural and dynamical properties revealed by a quantum mechanical charge field molecular dynamics study. *Journal of Computational Chemistry*, 31(2): 278–285, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alipour:2018:DMM

[Ali18] Mojtaba Alipour. Dipole moments of molecules with multireference character from optimally tuned range-separated density functional theory. *Journal of Computational Chemistry*, 39(20):1508–1516, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aidas:2015:AAP

[ALK+15] Kestutis Aidas, Kiril Lanevskij, Rytis Kubilius, Liutauras Juska, Daumantas Petkevicius, and Pranas Japertas. Aqueous acidities of primary benzenesulfonamides: Quantum chemical predictions based on density functional theory and SMD. *Journal of Computational Chemistry*, 36(29):2158–2167, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allouche:2011:GGU

[All11] Abdul-Rahman Allouche. Gabedit — a graphical user interface for computational chemistry softwares. *Journal of Computational Chemistry*, 32(1):174–182, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

AlQuraishi:2019:PNE

[AlQ19] Mohammed AlQuraishi. Parallelized natural extension reference frame: Parallelized conversion from internal to Cartesian coordinates. *Journal of Computational Chemistry*, 40(7):885–892, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aleksandrov:2018:CPD

[ALRM18] Alexey Aleksandrov, Fang-Yu Lin, Benoît Roux, and Alexander D. MacKerell Jr. Combining the polarizable Drude force field with a continuum electrostatic Poisson–Boltzmann implicit solvation model. *Journal of Computational Chemistry*, 39(22):1707–1719, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ai:2010:IBF

[ALW+10] Chunzhi Ai, Yan Li, Yonghua Wang, Wei Li, Peipei Dong, Guangbo Ge, and Ling Yang. Investigation of binding features: Effects on the interaction between CYP2A6 and inhibitors. *Journal of Computational Chemistry*, 31(9):1822–1831, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allen:2010:EAM

[AM10] Benjamin D. Allen and Stephen L. Mayo. An efficient algorithm for multistate protein design based on FASTER. *Journal of Computational Chemistry*, 31(5):904–916, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ariyarathna:2019:EGSa

[AM19a] Isuru R. Ariyarathna and Evangelos Miliordos. Electronic and geometric structure analysis of neutral and anionic alkali metal complexes of the CX series (X = O, S, Se, Te, Po): the case of M $(\mathrm{CX})_n = 1-4$ (M = Li, Na) and their dimers. *Journal of Computational Chemistry*, 40(13):1344–1351, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ariyarathna:2019:EGSb

[AM19b] Isuru R. Ariyarathna and Evangelos Miliordos. Electronic and geometric structure analysis of neutral and anionic metal nitric chalcogens: the case of MNX series (M = Li, Na, Be and X=O, S, Se, Te). *Journal of Computational Chemistry*, 40(19):1740–1751, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Al-Muhtaseb:2011:TSU

[AMAA+11] Ala'a H. Al-Muhtaseb, Mohammednoor Altarawneh, Mansour H. Almatarneh, Raymond A. Poirier, and Niveen W. Assaf. Theoretical study on the unimolecular decomposition of thiophenol. *Journal of Computational Chemistry*, 32(12):

2708–2715, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aguilar-Mogas:2010:IAB

[AMGB10] Antoni Aguilar-Mogas, Xavier Giménez, and Josep Maria Bofill. Implementation of an algorithm based on the Runge–Kutta–Fehlberg technique and the potential energy as a reaction coordinate to locate intrinsic reaction paths. *Journal of Computational Chemistry*, 31(13):2510–2525, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Addicoat:2011:DFT

[AMK11] Matthew A. Addicoat, Gregory F. Metha, and Tak W. Kee. Density functional theory investigation of Cu(I)- and Cu(II)-curcumin complexes. *Journal of Computational Chemistry*, 32 (3):429–438, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alberto:2014:ESI

[AMQ+14] Marta E. Alberto, Gloria Mazzone, Angelo D. Quartarolo, Flavio Fortes Ramos Sousa, Emilia Sicilia, and Nino Russo. Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. *Journal of Computational Chemistry*, 35 (29):2107–2113, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aquino:2011:CTS

[ANH+11] Adélia J. A. Aquino, Dana Nachtigallova, Pavel Hobza, Donald G. Truhlar, Christof Hättig, and Hans Lischka. The charge-transfer states in a stacked nucleobase dimer complex: a benchmark study. *Journal of Computational Chemistry*, 32 (7):1217–1227, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2010:CFE

[Ano10a] Anonymous. Computing free energy hypersurfaces for anisotropic intermolecular associations. *Journal of Computational Chemistry*, 31(6), April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2010:JCC

[Ano10b] Anonymous. Journal of Computational Chemistry, Volume 31, Number 2, January 30, 2010. *Journal of Computational Chemistry*, 31(6):1344, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2011:TAT

[Ano11] Anonymous. Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. *Journal of Computational Chemistry*, 32(2), January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIa

[Ano12a] Anonymous. Cover image: Inside cover, volume 33, issue 23. *Journal of Computational Chemistry*, 33(23):iii–iv, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIb

[Ano12b] Anonymous. Cover image: Inside cover, volume 33, issue 24. *Journal of Computational Chemistry*, 33(24):iii–iv, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIc

[Ano12c] Anonymous. Cover image: Inside cover, volume 33, issue 25. *Journal of Computational Chemistry*, 33(25):iii–iv, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIId

[Ano12d] Anonymous. Cover image: Inside cover, volume 33, issue 26. *Journal of Computational Chemistry*, 33(26):iii–iv, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIe

[Ano12e] Anonymous. Cover image: Inside cover, volume 33, issue 27. *Journal of Computational Chemistry*, 33(27):iii–iv, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIf

[Ano12f] Anonymous. Cover image: Inside cover, volume 33, issue 28. *Journal of Computational Chemistry*, 33(28):iii–iv, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIg

[Ano12g] Anonymous. Cover image: Inside cover, volume 33, issue 29. *Journal of Computational Chemistry*, 33(29):iii–iv, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIh

[Ano12h] Anonymous. Cover image: Inside cover, volume 33, issue 30. *Journal of Computational Chemistry*, 33(30):iii–iv, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIi

[Ano12i] Anonymous. Cover image: Inside cover, volume 33, issue 31. *Journal of Computational Chemistry*, 33(31):iii–iv, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIIj

[Ano12j] Anonymous. Cover image: Inside cover, volume 33, issue 32. *Journal of Computational Chemistry*, 33(32):iii–iv, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVa

[Ano12k] Anonymous. Cover image, volume 33, issue 23. *Journal of Computational Chemistry*, 33(23):i–ii, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVb

[Ano12l] Anonymous. Cover image, volume 33, issue 24. *Journal of Computational Chemistry*, 33(24):i–ii, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVc

[Ano12m] Anonymous. Cover image, volume 33, issue 25. *Journal of Computational Chemistry*, 33(25):i–ii, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVd

[Ano12n] Anonymous. Cover image, volume 33, issue 26. *Journal of Computational Chemistry*, 33(26):i–ii, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVe

[Ano12o] Anonymous. Cover image, volume 33, issue 27. *Journal of Computational Chemistry*, 33(27):i–ii, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVf

[Ano12p] Anonymous. Cover image, volume 33, issue 28. *Journal of Computational Chemistry*, 33(28):i–ii, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVg

[Ano12q] Anonymous. Cover image, volume 33, issue 29. *Journal of Computational Chemistry*, 33(29):i–ii, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVh

[Ano12r] Anonymous. Cover image, volume 33, issue 30. *Journal of Computational Chemistry*, 33(30):i–ii, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVi

[Ano12s] Anonymous. Cover image, volume 33, issue 31. *Journal of Computational Chemistry*, 33(31):i–ii, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:CIVj

[Ano12t] Anonymous. Cover image, volume 33, issue 32. *Journal of Computational Chemistry*, 33(32):i–ii, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2012:RPP

[Ano12u] Anonymous. Retracted: "Prediction of posttranslational modification sites from sequences with kernel methods" by Xiaobo Wang, Yongcui Wang, Yingjie Tian, Xiaojian Shao, Ling-Yun Wu, and Naiyang Deng, published online on 21 April 2010. *Journal of Computational Chemistry*, 33(17):1524, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIa

[Ano13a] Anonymous. Cover image: Inside cover, volume 34, issue 1. *Journal of Computational Chemistry*, 34(1):iii–iv, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIj

[Ano13b] Anonymous. Cover image: Inside cover, volume 34, issue 10. *Journal of Computational Chemistry*, 34(10):iii–iv, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIk

[Ano13c] Anonymous. Cover image: Inside cover, volume 34, issue 11. *Journal of Computational Chemistry*, 34(11):iii–iv, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIl

[Ano13d] Anonymous. Cover image: Inside cover, volume 34, issue 12. *Journal of Computational Chemistry*, 34(12):iii–iv, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIm

[Ano13e] Anonymous. Cover image: Inside cover, volume 34, issue 13. *Journal of Computational Chemistry*, 34(13):iii–iv, May 15,

2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIn

[Ano13f] Anonymous. Cover image: Inside cover, volume 34, issue 14. *Journal of Computational Chemistry*, 34(14):iii–iv, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIo

[Ano13g] Anonymous. Cover image: Inside cover, volume 34, issue 15. *Journal of Computational Chemistry*, 34(15):iii–iv, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIp

[Ano13h] Anonymous. Cover image: Inside cover, volume 34, issue 16. *Journal of Computational Chemistry*, 34(16):iii–iv, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIq

[Ano13i] Anonymous. Cover image: Inside cover, volume 34, issue 17. *Journal of Computational Chemistry*, 34(17):iii–iv, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIr

[Ano13j] Anonymous. Cover image: Inside cover, volume 34, issue 18. *Journal of Computational Chemistry*, 34(18):iii–iv, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIs

[Ano13k] Anonymous. Cover image: Inside cover, volume 34, issue 19. *Journal of Computational Chemistry*, 34(19):iii–iv, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIb

[Ano13l] Anonymous. Cover image: Inside cover, volume 34, issue 2. *Journal of Computational Chemistry*, 34(2):iii–iv, January 15,

2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIt

[Ano13m] Anonymous. Cover image: Inside cover, volume 34, issue 20. *Journal of Computational Chemistry*, 34(20):iii–iv, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIu

[Ano13n] Anonymous. Cover image: Inside cover, volume 34, issue 21. *Journal of Computational Chemistry*, 34(21):iii–iv, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIv

[Ano13o] Anonymous. Cover image: Inside cover, volume 34, issue 22. *Journal of Computational Chemistry*, 34(22):iii–iv, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIw

[Ano13p] Anonymous. Cover image: Inside cover, volume 34, issue 23. *Journal of Computational Chemistry*, 34(23):iii–iv, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIx

[Ano13q] Anonymous. Cover image: Inside cover, volume 34, issue 24. *Journal of Computational Chemistry*, 34(24):iii–iv, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIy

[Ano13r] Anonymous. Cover image: Inside cover, volume 34, issue 25. *Journal of Computational Chemistry*, 34(25):iii–iv, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIz

[Ano13s] Anonymous. Cover image: Inside cover, volume 34, issue 26. *Journal of Computational Chemistry*, 34(26):iii–iv, October 5,

2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIba

[Ano13t] Anonymous. Cover image: Inside cover, volume 34, issue 27. *Journal of Computational Chemistry*, 34(27):iii–iv, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbb

[Ano13u] Anonymous. Cover image: Inside cover, volume 34, issue 28. *Journal of Computational Chemistry*, 34(28):iii–iv, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbc

[Ano13v] Anonymous. Cover image: Inside cover, volume 34, issue 29. *Journal of Computational Chemistry*, 34(29):iii–iv, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIc

[Ano13w] Anonymous. Cover image: Inside cover, volume 34, issue 3. *Journal of Computational Chemistry*, 34(3):iii–iv, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbd

[Ano13x] Anonymous. Cover image: Inside cover, volume 34, issue 31. *Journal of Computational Chemistry*, 34(31):iii–iv, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIbe

[Ano13y] Anonymous. Cover image: Inside cover, volume 34, issue 32. *Journal of Computational Chemistry*, 34(32):iii–iv, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIId

[Ano13z] Anonymous. Cover image: Inside cover, volume 34, issue 4. *Journal of Computational Chemistry*, 34(4):iii–iv, February 5,

2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIe

[Ano13-27] Anonymous. Cover image: Inside cover, volume 34, issue 5. *Journal of Computational Chemistry*, 34(5):iii–iv, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIf

[Ano13-28] Anonymous. Cover image: Inside cover, volume 34, issue 6. *Journal of Computational Chemistry*, 34(6):iii–iv, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIg

[Ano13-29] Anonymous. Cover image: Inside cover, volume 34, issue 7. *Journal of Computational Chemistry*, 34(7):iii–iv, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIh

[Ano13-30] Anonymous. Cover image: Inside cover, volume 34, issue 8. *Journal of Computational Chemistry*, 34(8):iii–iv, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIIi

[Ano13-31] Anonymous. Cover image: Inside cover, volume 34, issue 9. *Journal of Computational Chemistry*, 34(9):iii–iv, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVa

[Ano13-32] Anonymous. Cover image, volume 34, issue 1. *Journal of Computational Chemistry*, 34(1):i–ii, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVj

[Ano13-33] Anonymous. Cover image, volume 34, issue 10. *Journal of Computational Chemistry*, 34(10):i–ii, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVk

[Ano13-34] Anonymous. Cover image, volume 34, issue 11. *Journal of Computational Chemistry*, 34(11):i–ii, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVl

[Ano13-35] Anonymous. Cover image, volume 34, issue 12. *Journal of Computational Chemistry*, 34(12):i–ii, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVm

[Ano13-36] Anonymous. Cover image, volume 34, issue 13. *Journal of Computational Chemistry*, 34(13):i–ii, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVn

[Ano13-37] Anonymous. Cover image, volume 34, issue 14. *Journal of Computational Chemistry*, 34(14):i–ii, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVo

[Ano13-38] Anonymous. Cover image, volume 34, issue 15. *Journal of Computational Chemistry*, 34(15):i–ii, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVp

[Ano13-39] Anonymous. Cover image, volume 34, issue 16. *Journal of Computational Chemistry*, 34(16):i–ii, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVq

[Ano13-40] Anonymous. Cover image, volume 34, issue 17. *Journal of Computational Chemistry*, 34(17):i–ii, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVr

[Ano13-41] Anonymous. Cover image, volume 34, issue 18. *Journal of Computational Chemistry*, 34(18):i–ii, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVs

[Ano13-42] Anonymous. Cover image, volume 34, issue 19. *Journal of Computational Chemistry*, 34(19):i–ii, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVb

[Ano13-43] Anonymous. Cover image, volume 34, issue 2. *Journal of Computational Chemistry*, 34(2):i–ii, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVt

[Ano13-44] Anonymous. Cover image, volume 34, issue 20. *Journal of Computational Chemistry*, 34(20):i–ii, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVu

[Ano13-45] Anonymous. Cover image, volume 34, issue 21. *Journal of Computational Chemistry*, 34(21):i–ii, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVv

[Ano13-46] Anonymous. Cover image, volume 34, issue 22. *Journal of Computational Chemistry*, 34(22):i–ii, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVw

[Ano13-47] Anonymous. Cover image, volume 34, issue 23. *Journal of Computational Chemistry*, 34(23):i–ii, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVx

[Ano13-48] Anonymous. Cover image, volume 34, issue 24. *Journal of Computational Chemistry*, 34(24):i–ii, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVy

[Ano13-49] Anonymous. Cover image, volume 34, issue 25. *Journal of Computational Chemistry*, 34(25):i–ii, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVz

[Ano13-50] Anonymous. Cover image, volume 34, issue 26. *Journal of Computational Chemistry*, 34(26):i–ii, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVba

[Ano13-51] Anonymous. Cover image, volume 34, issue 27. *Journal of Computational Chemistry*, 34(27):i–ii, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbb

[Ano13-52] Anonymous. Cover image, volume 34, issue 28. *Journal of Computational Chemistry*, 34(28):i–ii, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbc

[Ano13-53] Anonymous. Cover image, volume 34, issue 29. *Journal of Computational Chemistry*, 34(29):i–ii, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVc

[Ano13-54] Anonymous. Cover image, volume 34, issue 3. *Journal of Computational Chemistry*, 34(3):i–ii, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbd

[Ano13-55] Anonymous. Cover image, volume 34, issue 30. *Journal of Computational Chemistry*, 34(30):i–ii, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbe

[Ano13-56] Anonymous. Cover image, volume 34, issue 30. *Journal of Computational Chemistry*, 34(30):iii–iv, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbf

[Ano13-57] Anonymous. Cover image, volume 34, issue 31. *Journal of Computational Chemistry*, 34(31):i–ii, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVbg

[Ano13-58] Anonymous. Cover image, volume 34, issue 32. *Journal of Computational Chemistry*, 34(32):i–ii, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVd

[Ano13-59] Anonymous. Cover image, volume 34, issue 4. *Journal of Computational Chemistry*, 34(4):i–ii, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVe

[Ano13-60] Anonymous. Cover image, volume 34, issue 5. *Journal of Computational Chemistry*, 34(5):i–ii, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVf

[Ano13-61] Anonymous. Cover image, volume 34, issue 6. *Journal of Computational Chemistry*, 34(6):i–ii, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVg

[Ano13-62] Anonymous. Cover image, volume 34, issue 7. *Journal of Computational Chemistry*, 34(7):i–ii, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVh

[Ano13-63] Anonymous. Cover image, volume 34, issue 8. *Journal of Computational Chemistry*, 34(8):i–ii, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2013:CIVi

[Ano13-64] Anonymous. Cover image, volume 34, issue 9. *Journal of Computational Chemistry*, 34(9):i–ii, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CII

[Ano14a] Anonymous. Cover image: Inside cover, volume 35, issue 14. *Journal of Computational Chemistry*, 35(14):iii–iv, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVa

[Ano14b] Anonymous. Cover image, volume 35, issue 1. *Journal of Computational Chemistry*, 35(1):i–ii, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVb

[Ano14c] Anonymous. Cover image, volume 35, issue 1. *Journal of Computational Chemistry*, 35(1):iii–iv, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVx

[Ano14d] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):i–ii, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVy

[Ano14e] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):iii–iv, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVz

[Ano14f] Anonymous. Cover image, volume 35, issue 10. *Journal of Computational Chemistry*, 35(10):v–vi, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVba

[Ano14g] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):i–ii, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbb

[Ano14h] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):iii–iv, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbc

[Ano14i] Anonymous. Cover image, volume 35, issue 11. *Journal of Computational Chemistry*, 35(11):v–vi, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbd

[Ano14j] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):i–ii, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbe

[Ano14k] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):iii–iv, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbf

[Ano14l] Anonymous. Cover image, volume 35, issue 12. *Journal of Computational Chemistry*, 35(12):v–vi, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbg

[Ano14m] Anonymous. Cover image, volume 35, issue 13. *Journal of Computational Chemistry*, 35(13):i–ii, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbh

[Ano14n] Anonymous. Cover image, volume 35, issue 13. *Journal of Computational Chemistry*, 35(13):iii–iv, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbi

[Ano14o] Anonymous. Cover image, volume 35, issue 14. *Journal of Computational Chemistry*, 35(14):i–ii, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbj

[Ano14p] Anonymous. Cover image, volume 35, issue 15. *Journal of Computational Chemistry*, 35(15):i–ii, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbk

[Ano14q] Anonymous. Cover image, volume 35, issue 15. *Journal of Computational Chemistry*, 35(15):iii–iv, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbl

[Ano14r] Anonymous. Cover image, volume 35, issue 16. *Journal of Computational Chemistry*, 35(16):i–ii, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbm

[Ano14s] Anonymous. Cover image, volume 35, issue 16. *Journal of Computational Chemistry*, 35(16):iii–iv, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbn

[Ano14t] Anonymous. Cover image, volume 35, issue 17. *Journal of Computational Chemistry*, 35(17):i–ii, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbo

[Ano14u] Anonymous. Cover image, volume 35, issue 17. *Journal of Computational Chemistry*, 35(17):iii–iv, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbp

[Ano14v] Anonymous. Cover image, volume 35, issue 18. *Journal of Computational Chemistry*, 35(18):i–ii, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbq

[Ano14w] Anonymous. Cover image, volume 35, issue 18. *Journal of Computational Chemistry*, 35(18):iii–iv, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbr

[Ano14x] Anonymous. Cover image, volume 35, issue 19. *Journal of Computational Chemistry*, 35(19):i–ii, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbs

[Ano14y] Anonymous. Cover image, volume 35, issue 19. *Journal of Computational Chemistry*, 35(19):iii–iv, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVc

[Ano14z] Anonymous. Cover image, volume 35, issue 2. *Journal of Computational Chemistry*, 35(2):i–ii, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVd

[Ano14-27] Anonymous. Cover image, volume 35, issue 2. *Journal of Computational Chemistry*, 35(2):iii–iv, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbt

[Ano14-28] Anonymous. Cover image, volume 35, issue 20. *Journal of Computational Chemistry*, 35(20):i–ii, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbu

[Ano14-29] Anonymous. Cover image, volume 35, issue 20. *Journal of Computational Chemistry*, 35(20):iii–iv, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbv

[Ano14-30] Anonymous. Cover image, volume 35, issue 21. *Journal of Computational Chemistry*, 35(21):i–ii, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbw

[Ano14-31] Anonymous. Cover image, volume 35, issue 21. *Journal of Computational Chemistry*, 35(21):iii–iv, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbx

[Ano14-32] Anonymous. Cover image, volume 35, issue 22. *Journal of Computational Chemistry*, 35(22):i–ii, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVby

[Ano14-33] Anonymous. Cover image, volume 35, issue 22. *Journal of Computational Chemistry*, 35(22):iii–iv, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVbz

[Ano14-34] Anonymous. Cover image, volume 35, issue 23. *Journal of Computational Chemistry*, 35(23):i–ii, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVca

[Ano14-35] Anonymous. Cover image, volume 35, issue 23. *Journal of Computational Chemistry*, 35(23):iii–iv, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcb

[Ano14-36] Anonymous. Cover image, volume 35, issue 24. *Journal of Computational Chemistry*, 35(24):i–ii, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcc

[Ano14-37] Anonymous. Cover image, volume 35, issue 24. *Journal of Computational Chemistry*, 35(24):iii–iv, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcd

[Ano14-38] Anonymous. Cover image, volume 35, issue 25. *Journal of Computational Chemistry*, 35(25):i–ii, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVce

[Ano14-39] Anonymous. Cover image, volume 35, issue 25. *Journal of Computational Chemistry*, 35(25):iii–iv, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcf

[Ano14-40] Anonymous. Cover image, volume 35, issue 26. *Journal of Computational Chemistry*, 35(26):i–ii, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcg

[Ano14-41] Anonymous. Cover image, volume 35, issue 26. *Journal of Computational Chemistry*, 35(26):iii–iv, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVch

[Ano14-42] Anonymous. Cover image, volume 35, issue 27. *Journal of Computational Chemistry*, 35(27):i–ii, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVci

[Ano14-43] Anonymous. Cover image, volume 35, issue 27. *Journal of Computational Chemistry*, 35(27):iii–iv, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcj

[Ano14-44] Anonymous. Cover image, volume 35, issue 28. *Journal of Computational Chemistry*, 35(28):i–ii, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVck

[Ano14-45] Anonymous. Cover image, volume 35, issue 28. *Journal of Computational Chemistry*, 35(28):iii–iv, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcl

[Ano14-46] Anonymous. Cover image, volume 35, issue 29. *Journal of Computational Chemistry*, 35(29):i–ii, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcm

[Ano14-47] Anonymous. Cover image, volume 35, issue 29. *Journal of Computational Chemistry*, 35(29):iii–iv, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVe

[Ano14-48] Anonymous. Cover image, volume 35, issue 3. *Journal of Computational Chemistry*, 35(3):i–ii, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVf

[Ano14-49] Anonymous. Cover image, volume 35, issue 3. *Journal of Computational Chemistry*, 35(3):iii–iv, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcn

[Ano14-50] Anonymous. Cover image, volume 35, issue 30. *Journal of Computational Chemistry*, 35(30):i–ii, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVco

[Ano14-51] Anonymous. Cover image, volume 35, issue 30. *Journal of Computational Chemistry*, 35(30):iii–iv, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcp

[Ano14-52] Anonymous. Cover image, volume 35, issue 31. *Journal of Computational Chemistry*, 35(31):i–ii, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcq

[Ano14-53] Anonymous. Cover image, volume 35, issue 31. *Journal of Computational Chemistry*, 35(31):iii–iv, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcr

[Ano14-54] Anonymous. Cover image, volume 35, issue 32. *Journal of Computational Chemistry*, 35(32):i–ii, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVcs

[Ano14-55] Anonymous. Cover image, volume 35, issue 32. *Journal of Computational Chemistry*, 35(32):iii–iv, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVg

[Ano14-56] Anonymous. Cover image, volume 35, issue 4. *Journal of Computational Chemistry*, 35(4):i–ii, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVh

[Ano14-57] Anonymous. Cover image, volume 35, issue 4. *Journal of Computational Chemistry*, 35(4):iii–iv, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVi

[Ano14-58] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):i–ii, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVj

[Ano14-59] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):iii–iv, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVk

[Ano14-60] Anonymous. Cover image, volume 35, issue 5. *Journal of Computational Chemistry*, 35(5):v–vi, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVl

[Ano14-61] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):i–ii, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVm

[Ano14-62] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):iii–iv, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVn

[Ano14-63] Anonymous. Cover image, volume 35, issue 6. *Journal of Computational Chemistry*, 35(6):v–vi, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVo

[Ano14-64] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):i–ii, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVp

[Ano14-65] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):iii–iv, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVq

[Ano14-66] Anonymous. Cover image, volume 35, issue 7. *Journal of Computational Chemistry*, 35(7):iv–v, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVr

[Ano14-67] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):i–ii, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVs

[Ano14-68] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):iii–iv, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVt

[Ano14-69] Anonymous. Cover image, volume 35, issue 8. *Journal of Computational Chemistry*, 35(8):v–vi, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVu

[Ano14-70] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):i–ii, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVv

[Ano14-71] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):iii–iv, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2014:CIVw

[Ano14-72] Anonymous. Cover image, volume 35, issue 9. *Journal of Computational Chemistry*, 35(9):v–vi, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVa

[Ano15a] Anonymous. Cover image, volume 36, issue 1. *Journal of Computational Chemistry*, 36(1):i–ii, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVb

[Ano15b] Anonymous. Cover image, volume 36, issue 1. *Journal of Computational Chemistry*, 36(1):iii–iv, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVu

[Ano15c] Anonymous. Cover image, volume 36, issue 10. *Journal of Computational Chemistry*, 36(10):i–ii, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVv

[Ano15d] Anonymous. Cover image, volume 36, issue 10. *Journal of Computational Chemistry*, 36(10):iii–iv, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVw

[Ano15e] Anonymous. Cover image, volume 36, issue 10. *Journal of Computational Chemistry*, 36(10):v–vi, April 15, 2015. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVx

[Ano15f] Anonymous. Cover image, volume 36, issue 11. *Journal of Computational Chemistry*, 36(11):i–ii, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVy

[Ano15g] Anonymous. Cover image, volume 36, issue 11. *Journal of Computational Chemistry*, 36(11):iii–iv, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVz

[Ano15h] Anonymous. Cover image, volume 36, issue 11. *Journal of Computational Chemistry*, 36(11):v–vi, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVba

[Ano15i] Anonymous. Cover image, volume 36, issue 12. *Journal of Computational Chemistry*, 36(12):i–ii, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbb

[Ano15j] Anonymous. Cover image, volume 36, issue 12. *Journal of Computational Chemistry*, 36(12):iii–iv, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbc

[Ano15k] Anonymous. Cover image, volume 36, issue 13. *Journal of Computational Chemistry*, 36(13):i–ii, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbd

[Ano15l] Anonymous. Cover image, volume 36, issue 13. *Journal of Computational Chemistry*, 36(13):iii–iv, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbe

[Ano15m] Anonymous. Cover image, volume 36, issue 14. *Journal of Computational Chemistry*, 36(14):i–ii, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbf

[Ano15n] Anonymous. Cover image, volume 36, issue 14. *Journal of Computational Chemistry*, 36(14):iii–iv, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbg

[Ano15o] Anonymous. Cover image, volume 36, issue 15. *Journal of Computational Chemistry*, 36(15):i–ii, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbh

[Ano15p] Anonymous. Cover image, volume 36, issue 16. *Journal of Computational Chemistry*, 36(16):i–ii, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbi

[Ano15q] Anonymous. Cover image, volume 36, issue 16. *Journal of Computational Chemistry*, 36(16):iii–iv, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbj

[Ano15r] Anonymous. Cover image, volume 36, issue 17. *Journal of Computational Chemistry*, 36(17):i–ii, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbk

[Ano15s] Anonymous. Cover image, volume 36, issue 18. *Journal of Computational Chemistry*, 36(18):i–ii, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbl

[Ano15t] Anonymous. Cover image, volume 36, issue 18. *Journal of Computational Chemistry*, 36(18):iii–iv, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbm

[Ano15u] Anonymous. Cover image, volume 36, issue 19. *Journal of Computational Chemistry*, 36(19):i–ii, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVc

[Ano15v] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):i–ii, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVd

[Ano15w] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):iii–iv, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVe

[Ano15x] Anonymous. Cover image, volume 36, issue 2. *Journal of Computational Chemistry*, 36(2):v–vi, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbn

[Ano15y] Anonymous. Cover image, volume 36, issue 20. *Journal of Computational Chemistry*, 36(20):i–ii, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbo

[Ano15z] Anonymous. Cover image, volume 36, issue 21. *Journal of Computational Chemistry*, 36(21):i–ii, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbp

[Ano15-27] Anonymous. Cover image, volume 36, issue 22. *Journal of Computational Chemistry*, 36(22):i–ii, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbq

[Ano15-28] Anonymous. Cover image, volume 36, issue 22. *Journal of Computational Chemistry*, 36(22):iii–iv, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbr

[Ano15-29] Anonymous. Cover image, volume 36, issue 23. *Journal of Computational Chemistry*, 36(23):i–ii, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbs

[Ano15-30] Anonymous. Cover image, volume 36, issue 24. *Journal of Computational Chemistry*, 36(24):i–ii, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbt

[Ano15-31] Anonymous. Cover image, volume 36, issue 25. *Journal of Computational Chemistry*, 36(25):i–ii, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbu

[Ano15-32] Anonymous. Cover image, volume 36, issue 26. *Journal of Computational Chemistry*, 36(26):i–ii, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbv

[Ano15-33] Anonymous. Cover image, volume 36, issue 26. *Journal of Computational Chemistry*, 36(26):iii–iv, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbw

[Ano15-34] Anonymous. Cover image, volume 36, issue 27. *Journal of Computational Chemistry*, 36(27):i–ii, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbx

[Ano15-35] Anonymous. Cover image, volume 36, issue 28. *Journal of Computational Chemistry*, 36(28):i–ii, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVby

[Ano15-36] Anonymous. Cover image, volume 36, issue 29. *Journal of Computational Chemistry*, 36(29):i–ii, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVf

[Ano15-37] Anonymous. Cover image, volume 36, issue 3. *Journal of Computational Chemistry*, 36(3):i–ii, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVg

[Ano15-38] Anonymous. Cover image, volume 36, issue 3. *Journal of Computational Chemistry*, 36(3):iii–iv, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVbz

[Ano15-39] Anonymous. Cover image, volume 36, issue 30. *Journal of Computational Chemistry*, 36(30):i–ii, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVca

[Ano15-40] Anonymous. Cover image, volume 36, issue 30. *Journal of Computational Chemistry*, 36(30):iii–iv, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVcb

[Ano15-41] Anonymous. Cover image, volume 36, issue 31. *Journal of Computational Chemistry*, 36(31):i–ii, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVcc

[Ano15-42] Anonymous. Cover image, volume 36, issue 31. *Journal of Computational Chemistry*, 36(31):iii–iv, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVcd

[Ano15-43] Anonymous. Cover image, volume 36, issue 31. *Journal of Computational Chemistry*, 36(31):v–vi, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVce

[Ano15-44] Anonymous. Cover image, volume 36, issue 32. *Journal of Computational Chemistry*, 36(32):i–ii, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVh

[Ano15-45] Anonymous. Cover image, volume 36, issue 4. *Journal of Computational Chemistry*, 36(4):i–ii, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVi

[Ano15-46] Anonymous. Cover image, volume 36, issue 4. *Journal of Computational Chemistry*, 36(4):iii–iv, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVj

[Ano15-47] Anonymous. Cover image, volume 36, issue 5. *Journal of Computational Chemistry*, 36(5):i–ii, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVk

[Ano15-48] Anonymous. Cover image, volume 36, issue 5. *Journal of Computational Chemistry*, 36(5):iii–iv, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVl

[Ano15-49] Anonymous. Cover image, volume 36, issue 5. *Journal of Computational Chemistry*, 36(5):v–vi, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVm

[Ano15-50] Anonymous. Cover image, volume 36, issue 6. *Journal of Computational Chemistry*, 36(6):i–ii, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVn

[Ano15-51] Anonymous. Cover image, volume 36, issue 6. *Journal of Computational Chemistry*, 36(6):iii–iv, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVo

[Ano15-52] Anonymous. Cover image, volume 36, issue 7. *Journal of Computational Chemistry*, 36(7):i–ii, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVp

[Ano15-53] Anonymous. Cover image, volume 36, issue 7. *Journal of Computational Chemistry*, 36(7):iii–iv, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVq

[Ano15-54] Anonymous. Cover image, volume 36, issue 8. *Journal of Computational Chemistry*, 36(8):i–ii, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVr

[Ano15-55] Anonymous. Cover image, volume 36, issue 8. *Journal of Computational Chemistry*, 36(8):iii–iv, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVs

[Ano15-56] Anonymous. Cover image, volume 36, issue 9. *Journal of Computational Chemistry*, 36(9):i–ii, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:CIVt

[Ano15-57] Anonymous. Cover image, volume 36, issue 9. *Journal of Computational Chemistry*, 36(9):iii–iv, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2015:ECS

[Ano15-58] Anonymous. Erratum: Corrigendum: A spherical harmonic transform spectral analysis of a localized surface plasmon on a gold nano shell. *Journal of Computational Chemistry*, 36(2): 136, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [BH14].

Anonymous:2015:ECG

[Ano15-59] Anonymous. Erratum to Csonka, G. I., Nguyen, N. A., & Kolossváry, I. (1997). Simple tests for density functional methods. Journal of Computational Chemistry, 18 (12), 1534–1545. (DOI: `c7rfjv`). *Journal of Computational Chemistry*, 36(30):2270, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [CNK97].

Anonymous:2015:OPS

[Ano15-60] Anonymous. Obituary: Paul Schleyer 1930–2014. *Journal of Computational Chemistry*, 36(7):423, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVa

[Ano16a] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):i, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVb

[Ano16b] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):ii, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVc

[Ano16c] Anonymous. Cover image, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):iii, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVv

[Ano16d] Anonymous. Cover image, volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):i, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVw

[Ano16e] Anonymous. Cover image, volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):ii, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVx

[Ano16f] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):i, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVy

[Ano16g] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):ii, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVz

[Ano16h] Anonymous. Cover image, volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):iii, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVba

[Ano16i] Anonymous. Cover image, volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):i, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbb

[Ano16j] Anonymous. Cover image, volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):ii, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbc

[Ano16k] Anonymous. Cover image, volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):i–ii, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbd

[Ano16l] Anonymous. Cover image, volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):i–ii, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbe

[Ano16m] Anonymous. Cover image, volume 37, issue 15. *Journal of Computational Chemistry*, 37(15):i, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbf

[Ano16n] Anonymous. Cover image, volume 37, issue 15. *Journal of Computational Chemistry*, 37(15):ii, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbg

[Ano16o] Anonymous. Cover image, volume 37, issue 16. *Journal of Computational Chemistry*, 37(16):i, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbh

[Ano16p] Anonymous. Cover image, volume 37, issue 17. *Journal of Computational Chemistry*, 37(17):i, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbi

[Ano16q] Anonymous. Cover image, volume 37, issue 18. *Journal of Computational Chemistry*, 37(18):i, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbj

[Ano16r] Anonymous. Cover image, volume 37, issue 19. *Journal of Computational Chemistry*, 37(19):i, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVd

[Ano16s] Anonymous. Cover image, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):i, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVe

[Ano16t] Anonymous. Cover image, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):ii, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbk

[Ano16u] Anonymous. Cover image, volume 37, issue 20. *Journal of Computational Chemistry*, 37(20):i, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbl

[Ano16v] Anonymous. Cover image, volume 37, issue 21. *Journal of Computational Chemistry*, 37(21):i, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbm

[Ano16w] Anonymous. Cover image, volume 37, issue 21. *Journal of Computational Chemistry*, 37(21):ii, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbn

[Ano16x] Anonymous. Cover image, volume 37, issue 22. *Journal of Computational Chemistry*, 37(22):i, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbo

[Ano16y] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):i, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbp

[Ano16z] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):ii, September 5, 2016. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbq

[Ano16-27] Anonymous. Cover image, volume 37, issue 23. *Journal of Computational Chemistry*, 37(23):iii, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbr

[Ano16-28] Anonymous. Cover image, volume 37, issue 24. *Journal of Computational Chemistry*, 37(24):i, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbs

[Ano16-29] Anonymous. Cover image, volume 37, issue 24. *Journal of Computational Chemistry*, 37(24):ii, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbt

[Ano16-30] Anonymous. Cover image, volume 37, issue 25. *Journal of Computational Chemistry*, 37(25):i, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbu

[Ano16-31] Anonymous. Cover image, volume 37, issue 25. *Journal of Computational Chemistry*, 37(25):ii, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbv

[Ano16-32] Anonymous. Cover image, volume 37, issue 26. *Journal of Computational Chemistry*, 37(26):i, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbw

[Ano16-33] Anonymous. Cover image, volume 37, issue 26. *Journal of Computational Chemistry*, 37(26):ii, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbx

[Ano16-34] Anonymous. Cover image, volume 37, issue 27. *Journal of Computational Chemistry*, 37(27):i, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVby

[Ano16-35] Anonymous. Cover image, volume 37, issue 28. *Journal of Computational Chemistry*, 37(28):i, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVbz

[Ano16-36] Anonymous. Cover image, volume 37, issue 29. *Journal of Computational Chemistry*, 37(29):i, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVf

[Ano16-37] Anonymous. Cover image, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):i, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVg

[Ano16-38] Anonymous. Cover image, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):ii, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVca

[Ano16-39] Anonymous. Cover image, volume 37, issue 30. *Journal of Computational Chemistry*, 37(30):i, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVcb

[Ano16-40] Anonymous. Cover image, volume 37, issue 31. *Journal of Computational Chemistry*, 37(31):i, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVcc

[Ano16-41] Anonymous. Cover image, volume 37, issue 32. *Journal of Computational Chemistry*, 37(32):i, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVh

[Ano16-42] Anonymous. Cover image, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):i, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVi

[Ano16-43] Anonymous. Cover image, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):ii, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVj

[Ano16-44] Anonymous. Cover image, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):i, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVk

[Ano16-45] Anonymous. Cover image, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):ii, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVl

[Ano16-46] Anonymous. Cover image, volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):i, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVm

[Ano16-47] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):i, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVn

[Ano16-48] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):ii, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVo

[Ano16-49] Anonymous. Cover image, volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):iii, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVp

[Ano16-50] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):i, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVq

[Ano16-51] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):ii, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVr

[Ano16-52] Anonymous. Cover image, volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):iii, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVs

[Ano16-53] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):i, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVt

[Ano16-54] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):ii, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:CIVu

[Ano16-55] Anonymous. Cover image, volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):iii, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:EPR

[Ano16-56] Anonymous. Editorial: Paul Von Ragué Schleyer (1930–2014). *Journal of Computational Chemistry*, 37(1):9, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIa

[Ano16-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(15):1329–1333, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIb

[Ano16-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(16):1407–1412, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IId

[Ano16-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(17):1525–1530, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIf

[Ano16-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(18):1651–1656, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIg

[Ano16-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(19):1747, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIh

[Ano16-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(20):1855, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIi

[Ano16-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(21):1947–1952, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIj

[Ano16-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(22):2039–2043, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIk

[Ano16-65] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(23):2119–2123, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIl

[Ano16-66] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(24):2165–2169, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIm

[Ano16-67] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(25):2243–2247, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIn

[Ano16-68] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(26):2335–2339, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIo

[Ano16-69] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(27):2403–2407, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIp

[Ano16-70] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(28):2479–2483, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIq

[Ano16-71] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(29):2547–2551, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIr

[Ano16-72] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(30):2617–2621, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIs

[Ano16-73] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(31):2671, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIu

[Ano16-74] Anonymous. Issue information. *Journal of Computational Chemistry*, 37(32):2743–2747, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICa

[Ano16-75] Anonymous. Issue information — coming soon, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):1, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICs

[Ano16-76] Anonymous. Issue information — coming soon: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):871, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICu

[Ano16-77] Anonymous. Issue information — coming soon: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):955, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICw

[Ano16-78] Anonymous. Issue information — coming soon: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1037, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICy

[Ano16-79] Anonymous. Issue information — coming soon: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1133, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICba

[Ano16-80] Anonymous. Issue information — coming soon: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1245, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICc

[Ano16-81] Anonymous. Issue information — coming soon, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):155, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICe

[Ano16-82] Anonymous. Issue information — coming soon, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):315, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICg

[Ano16-83] Anonymous. Issue information — coming soon, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):389, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICi

[Ano16-84] Anonymous. Issue information — coming soon, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):461, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICk

[Ano16-85] Anonymous. Issue information — coming soon: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):543, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICm

[Ano16-86] Anonymous. Issue information — coming soon: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):623, March

15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICo

[Ano16-87] Anonymous. Issue information — coming soon: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):695, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICq

[Ano16-88] Anonymous. Issue information — coming soon: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):781, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICb

[Ano16-89] Anonymous. Issue information — copyright, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):2, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICt

[Ano16-90] Anonymous. Issue information — copyright: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10):872, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICv

[Ano16-91] Anonymous. Issue information — copyright: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11):956, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICx

[Ano16-92] Anonymous. Issue information — copyright: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1038, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICz

[Ano16-93] Anonymous. Issue information — copyright: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1134, May

15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICbb

[Ano16-94] Anonymous. Issue information — copyright: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1246, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICd

[Ano16-95] Anonymous. Issue information — copyright, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):156, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICf

[Ano16-96] Anonymous. Issue information — copyright, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):316, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICh

[Ano16-97] Anonymous. Issue information — copyright, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):390, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICj

[Ano16-98] Anonymous. Issue information — copyright, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):462, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICl

[Ano16-99] Anonymous. Issue information — copyright: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):544, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICn

[Ano16-100] Anonymous. Issue information — copyright: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):624, March 15,

2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICp

[Ano16-101] Anonymous. Issue information — copyright: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):696, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IICr

[Ano16-102] Anonymous. Issue information — copyright: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):782, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEj

[Ano16-103] Anonymous. Issue information — editorial board: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10): 873, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEk

[Ano16-104] Anonymous. Issue information — editorial board: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11): 957, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEl

[Ano16-105] Anonymous. Issue information — editorial board: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12):1039, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEm

[Ano16-106] Anonymous. Issue information — editorial board: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13):1135, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEn

[Ano16-107] Anonymous. Issue information — editorial board: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14):1247, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEb

[Ano16-108] Anonymous. Issue information — Editorial Board, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):157, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEc

[Ano16-109] Anonymous. Issue information — Editorial Board, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):317, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEd

[Ano16-110] Anonymous. Issue information — Editorial Board, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):391, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEf

[Ano16-111] Anonymous. Issue information — Editorial Board: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):545, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEg

[Ano16-112] Anonymous. Issue information — Editorial Board: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):625, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEh

[Ano16-113] Anonymous. Issue information — Editorial Board: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):697, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEi

[Ano16-114] Anonymous. Issue information — Editorial Board: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):783, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITa

[Ano16-115] Anonymous. Issue information — table of contents volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):4–8, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITj

[Ano16-116] Anonymous. Issue information — table of contents: Volume 37, issue 10. *Journal of Computational Chemistry*, 37(10): 874–875, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITk

[Ano16-117] Anonymous. Issue information — table of contents: Volume 37, issue 11. *Journal of Computational Chemistry*, 37(11): 958–959, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITl

[Ano16-118] Anonymous. Issue information — table of contents: Volume 37, issue 12. *Journal of Computational Chemistry*, 37(12): 1040–1042, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITm

[Ano16-119] Anonymous. Issue information — table of contents: Volume 37, issue 13. *Journal of Computational Chemistry*, 37(13): 1136–1138, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITn

[Ano16-120] Anonymous. Issue information — table of contents: Volume 37, issue 14. *Journal of Computational Chemistry*, 37(14): 1248–1250, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITb

[Ano16-121] Anonymous. Issue information — table of contents, volume 37, issue 2. *Journal of Computational Chemistry*, 37(2):158–

161, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITc

[Ano16-122] Anonymous. Issue information — table of contents, volume 37, issue 3. *Journal of Computational Chemistry*, 37(3):318–319, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITd

[Ano16-123] Anonymous. Issue information — table of contents, volume 37, issue 4. *Journal of Computational Chemistry*, 37(4):392–393, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITe

[Ano16-124] Anonymous. Issue information — table of contents, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):464–465, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITf

[Ano16-125] Anonymous. Issue information — table of contents: Volume 37, issue 6. *Journal of Computational Chemistry*, 37(6):546–548, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITg

[Ano16-126] Anonymous. Issue information — table of contents: Volume 37, issue 7. *Journal of Computational Chemistry*, 37(7):626–627, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITh

[Ano16-127] Anonymous. Issue information — table of contents: Volume 37, issue 8. *Journal of Computational Chemistry*, 37(8):698–699, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IITi

[Ano16-128] Anonymous. Issue information — table of contents: Volume 37, issue 9. *Journal of Computational Chemistry*, 37(9):

784–785, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEa

[Ano16-129] Anonymous. Issue information – Editorial Board, volume 37, issue 1. *Journal of Computational Chemistry*, 37(1):3, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2016:IIEe

[Ano16-130] Anonymous. Issue information – Editorial Board, volume 37, issue 5. *Journal of Computational Chemistry*, 37(5):463, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVa

[Ano17a] Anonymous. Cover image, volume 38, issue 1. *Journal of Computational Chemistry*, 38(1):i, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVj

[Ano17b] Anonymous. Cover image, volume 38, issue 10. *Journal of Computational Chemistry*, 38(10):i, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVk

[Ano17c] Anonymous. Cover image, volume 38, issue 11. *Journal of Computational Chemistry*, 38(11):i, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVl

[Ano17d] Anonymous. Cover image, volume 38, issue 12. *Journal of Computational Chemistry*, 38(12):i, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVm

[Ano17e] Anonymous. Cover image, volume 38, issue 13. *Journal of Computational Chemistry*, 38(13):i, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVn

[Ano17f] Anonymous. Cover image, volume 38, issue 14. *Journal of Computational Chemistry*, 38(14):i, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVo

[Ano17g] Anonymous. Cover image, volume 38, issue 15. *Journal of Computational Chemistry*, 38(15):i, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVp

[Ano17h] Anonymous. Cover image, volume 38, issue 15. *Journal of Computational Chemistry*, 38(15):ii, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVq

[Ano17i] Anonymous. Cover image, volume 38, issue 16. *Journal of Computational Chemistry*, 38(16):i, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVr

[Ano17j] Anonymous. Cover image, volume 38, issue 16. *Journal of Computational Chemistry*, 38(16):ii, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVs

[Ano17k] Anonymous. Cover image, volume 38, issue 17. *Journal of Computational Chemistry*, 38(17):i, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVt

[Ano17l] Anonymous. Cover image, volume 38, issue 18. *Journal of Computational Chemistry*, 38(18):i, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVu

[Ano17m] Anonymous. Cover image, volume 38, issue 19. *Journal of Computational Chemistry*, 38(19):i, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVb

[Ano17n] Anonymous. Cover image, volume 38, issue 2. *Journal of Computational Chemistry*, 38(2):i, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVv

[Ano17o] Anonymous. Cover image, volume 38, issue 20. *Journal of Computational Chemistry*, 38(20):i, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVw

[Ano17p] Anonymous. Cover image, volume 38, issue 21. *Journal of Computational Chemistry*, 38(21):i, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVx

[Ano17q] Anonymous. Cover image, volume 38, issue 22. *Journal of Computational Chemistry*, 38(22):i, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVy

[Ano17r] Anonymous. Cover image, volume 38, issue 23. *Journal of Computational Chemistry*, 38(23):i, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVz

[Ano17s] Anonymous. Cover image, volume 38, issue 24. *Journal of Computational Chemistry*, 38(24):i, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVba

[Ano17t] Anonymous. Cover image, volume 38, issue 25. *Journal of Computational Chemistry*, 38(25):i, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbb

[Ano17u] Anonymous. Cover image, volume 38, issue 26. *Journal of Computational Chemistry*, 38(26):i, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbc

[Ano17v] Anonymous. Cover image, volume 38, issue 27. *Journal of Computational Chemistry*, 38(27):i, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbd

[Ano17w] Anonymous. Cover image, volume 38, issue 28. *Journal of Computational Chemistry*, 38(28):i, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbe

[Ano17x] Anonymous. Cover image, volume 38, issue 29. *Journal of Computational Chemistry*, 38(29):i, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVc

[Ano17y] Anonymous. Cover image, volume 38, issue 3. *Journal of Computational Chemistry*, 38(3):i, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbf

[Ano17z] Anonymous. Cover image, volume 38, issue 30. *Journal of Computational Chemistry*, 38(30):i, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbg

[Ano17-27] Anonymous. Cover image, volume 38, issue 31. *Journal of Computational Chemistry*, 38(31):i, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVbh

[Ano17-28] Anonymous. Cover image, volume 38, issue 32. *Journal of Computational Chemistry*, 38(32):i, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVd

[Ano17-29] Anonymous. Cover image, volume 38, issue 4. *Journal of Computational Chemistry*, 38(4):i, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVe

[Ano17-30] Anonymous. Cover image, volume 38, issue 5. *Journal of Computational Chemistry*, 38(5):i, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVf

[Ano17-31] Anonymous. Cover image, volume 38, issue 6. *Journal of Computational Chemistry*, 38(6):i, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVg

[Ano17-32] Anonymous. Cover image, volume 38, issue 7. *Journal of Computational Chemistry*, 38(7):i, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVh

[Ano17-33] Anonymous. Cover image, volume 38, issue 8. *Journal of Computational Chemistry*, 38(8):i, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:CIVi

[Ano17-34] Anonymous. Cover image, volume 38, issue 9. *Journal of Computational Chemistry*, 38(9):i, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:E

[Ano17-35] Anonymous. Erratum. *Journal of Computational Chemistry*, 38(13):1015, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIa

[Ano17-36] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(1):1–5, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIb

[Ano17-37] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(2):59–63, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIc

[Ano17-38] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(3):127–131, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IId

[Ano17-39] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(4):189–193, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIe

[Ano17-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(5):251–255, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIf

[Ano17-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(6):313–317, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIg

[Ano17-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(7):395–399, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIh

[Ano17-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(8):475–479, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIi

[Ano17-44] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(9):563–567, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIj

[Ano17-45] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(10):639–644, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIk

[Ano17-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(11):767–771, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIl

[Ano17-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(12):855–859, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIm

[Ano17-48] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(13):935–939, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIn

[Ano17-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(14):1017–1021, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIo

[Ano17-50] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(15):1103–1110, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIp

[Ano17-51] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(16):1283–1290, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIq

[Ano17-52] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(17):1489–1494, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIr

[Ano17-53] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(18):1561–1565, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIs

[Ano17-54] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(19):1655–1659, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIt

[Ano17-55] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(20):1741–1745, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIu

[Ano17-56] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(21):1819–1823, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIv

[Ano17-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(22):1891–1895, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIw

[Ano17-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(23):1981–1986, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIx

[Ano17-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(24):2057–2061, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIy

[Ano17-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(25):2135–2139, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIz

[Ano17-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(26):2207–2211, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIba

[Ano17-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(27):2283–2287, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbb

[Ano17-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(28):2365–2369, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbc

[Ano17-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(29):2453–2457, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbd

[Ano17-65] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(30):2553–2557, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbe

[Ano17-66] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(31):2665–2670, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2017:IIbf

[Ano17-67] Anonymous. Issue information. *Journal of Computational Chemistry*, 38(32):2747–2751, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVa

[Ano18a] Anonymous. Cover image, volume 39, issue 1. *Journal of Computational Chemistry*, 39(1):i, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVb

[Ano18b] Anonymous. Cover image, volume 39, issue 1. *Journal of Computational Chemistry*, 39(1):ii, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVk

[Ano18c] Anonymous. Cover image, volume 39, issue 10. *Journal of Computational Chemistry*, 39(10):i, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVl

[Ano18d] Anonymous. Cover image, volume 39, issue 10. *Journal of Computational Chemistry*, 39(10):ii, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVm

[Ano18e] Anonymous. Cover image, volume 39, issue 11. *Journal of Computational Chemistry*, 39(11):i, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVn

[Ano18f] Anonymous. Cover image, volume 39, issue 12. *Journal of Computational Chemistry*, 39(12):i, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVo

[Ano18g] Anonymous. Cover image, volume 39, issue 13. *Journal of Computational Chemistry*, 39(13):i, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVp

[Ano18h] Anonymous. Cover image, volume 39, issue 14. *Journal of Computational Chemistry*, 39(14):i, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVq

[Ano18i] Anonymous. Cover image, volume 39, issue 15. *Journal of Computational Chemistry*, 39(15):i, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVr

[Ano18j] Anonymous. Cover image, volume 39, issue 16. *Journal of Computational Chemistry*, 39(16):i, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVs

[Ano18k] Anonymous. Cover image, volume 39, issue 17. *Journal of Computational Chemistry*, 39(17):i, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVt

[Ano18l] Anonymous. Cover image, volume 39, issue 18. *Journal of Computational Chemistry*, 39(18):i, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVu

[Ano18m] Anonymous. Cover image, volume 39, issue 19. *Journal of Computational Chemistry*, 39(19):i, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVc

[Ano18n] Anonymous. Cover image, volume 39, issue 2. *Journal of Computational Chemistry*, 39(2):i, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVv

[Ano18o] Anonymous. Cover image, volume 39, issue 20. *Journal of Computational Chemistry*, 39(20):1, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVw

[Ano18p] Anonymous. Cover image, volume 39, issue 20. *Journal of Computational Chemistry*, 39(20):1, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVx

[Ano18q] Anonymous. Cover image, volume 39, issue 21. *Journal of Computational Chemistry*, 39(21):C1, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVy

[Ano18r] Anonymous. Cover image, volume 39, issue 21. *Journal of Computational Chemistry*, 39(21):C2, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVz

[Ano18s] Anonymous. Cover image, volume 39, issue 22. *Journal of Computational Chemistry*, 39(22):C1, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVba

[Ano18t] Anonymous. Cover image, volume 39, issue 22. *Journal of Computational Chemistry*, 39(22):C2, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbb

[Ano18u] Anonymous. Cover image, volume 39, issue 23. *Journal of Computational Chemistry*, 39(23):C1, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbc

[Ano18v] Anonymous. Cover image, volume 39, issue 23. *Journal of Computational Chemistry*, 39(23):C2, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbd

[Ano18w] Anonymous. Cover image, volume 39, issue 24. *Journal of Computational Chemistry*, 39(24):C1, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbe

[Ano18x] Anonymous. Cover image, volume 39, issue 25. *Journal of Computational Chemistry*, 39(25):C1, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbf

[Ano18y] Anonymous. Cover image, volume 39, issue 26. *Journal of Computational Chemistry*, 39(26):C1, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbg

[Ano18z] Anonymous. Cover image, volume 39, issue 27. *Journal of Computational Chemistry*, 39(27):C1, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbh

[Ano18-27] Anonymous. Cover image, volume 39, issue 28. *Journal of Computational Chemistry*, 39(28):C1, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbi

[Ano18-28] Anonymous. Cover image, volume 39, issue 29. *Journal of Computational Chemistry*, 39(29):C1, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVd

[Ano18-29] Anonymous. Cover image, volume 39, issue 3. *Journal of Computational Chemistry*, 39(3):i, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbj

[Ano18-30] Anonymous. Cover image, volume 39, issue 30. *Journal of Computational Chemistry*, 39(30):C1, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbk

[Ano18-31] Anonymous. Cover image, volume 39, issue 31. *Journal of Computational Chemistry*, 39(31):C1, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVbl

[Ano18-32] Anonymous. Cover image, volume 39, issue 32. *Journal of Computational Chemistry*, 39(32):C1, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVe

[Ano18-33] Anonymous. Cover image, volume 39, issue 4. *Journal of Computational Chemistry*, 39(4):i, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVf

[Ano18-34] Anonymous. Cover image, volume 39, issue 5. *Journal of Computational Chemistry*, 39(5):i, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVg

[Ano18-35] Anonymous. Cover image, volume 39, issue 6. *Journal of Computational Chemistry*, 39(6):i, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVh

[Ano18-36] Anonymous. Cover image, volume 39, issue 7. *Journal of Computational Chemistry*, 39(7):i, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVi

[Ano18-37] Anonymous. Cover image, volume 39, issue 8. *Journal of Computational Chemistry*, 39(8):i, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:CIVj

[Ano18-38] Anonymous. Cover image, volume 39, issue 9. *Journal of Computational Chemistry*, 39(9):i, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIa

[Ano18-39] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(1):1–5, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIb

[Ano18-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(2):65–69, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIc

[Ano18-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(3):139–142, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IId

[Ano18-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(4):187–190, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIe

[Ano18-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(5):251–254, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIf

[Ano18-44] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(6):287–291, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIg

[Ano18-45] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(7):339–342, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIh

[Ano18-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(8):381–385, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIi

[Ano18-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(9):451–455, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIj

[Ano18-48] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(10):521–525, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIk

[Ano18-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(11):615–619, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIl

[Ano18-50] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(12):699–703, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIm

[Ano18-51] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(13):757–761, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIn

[Ano18-52] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(14):815–819, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIo

[Ano18-53] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(15):869–873, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIp

[Ano18-54] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(16):925–929, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIq

[Ano18-55] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(17):1013–1017, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIr

[Ano18-56] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(18):1077–1081, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIs

[Ano18-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(19):1169–1176, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIt

[Ano18-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(20):1359–1366, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIu

[Ano18-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(21):1579–1584, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIv

[Ano18-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(22):1691–1696, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIw

[Ano18-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(23):1829–1834, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIx

[Ano18-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(25):2033–2038, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIy

[Ano18-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(26):2147–2151, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIz

[Ano18-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(27):2263–2267, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIba

[Ano18-65] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(28):2345–2349, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIbb

[Ano18-66] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(29):2415–2419, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIbc

[Ano18-67] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(30):2489–2493, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIbd

[Ano18-68] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(31):2559–2563, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2018:IIbe

[Ano18-69] Anonymous. Issue information. *Journal of Computational Chemistry*, 39(32):2619–2623, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVa

[Ano19a] Anonymous. Cover image, volume 40, issue 1. *Journal of Computational Chemistry*, 40(1):C1, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVj

[Ano19b] Anonymous. Cover image, volume 40, issue 10. *Journal of Computational Chemistry*, 40(10):C1, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVk

[Ano19c] Anonymous. Cover image, volume 40, issue 11. *Journal of Computational Chemistry*, 40(11):C1, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVl

[Ano19d] Anonymous. Cover image, volume 40, issue 12. *Journal of Computational Chemistry*, 40(12):C1, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVm

[Ano19e] Anonymous. Cover image, volume 40, issue 13. *Journal of Computational Chemistry*, 40(13):C1, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVn

[Ano19f] Anonymous. Cover image, volume 40, issue 14. *Journal of Computational Chemistry*, 40(14):C1, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVo

[Ano19g] Anonymous. Cover image, volume 40, issue 15. *Journal of Computational Chemistry*, 40(15):C1, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVp

[Ano19h] Anonymous. Cover image, volume 40, issue 16. *Journal of Computational Chemistry*, 40(16):C1, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVq

[Ano19i] Anonymous. Cover image, volume 40, issue 17. *Journal of Computational Chemistry*, 40(17):C1, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVr

[Ano19j] Anonymous. Cover image, volume 40, issue 18. *Journal of Computational Chemistry*, 40(18):C1, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVs

[Ano19k] Anonymous. Cover image, volume 40, issue 19. *Journal of Computational Chemistry*, 40(19):C1, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVb

[Ano19l] Anonymous. Cover image, volume 40, issue 2. *Journal of Computational Chemistry*, 40(2):C1, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVt

[Ano19m] Anonymous. Cover image, volume 40, issue 20. *Journal of Computational Chemistry*, 40(20):C1, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVu

[Ano19n] Anonymous. Cover image, volume 40, issue 21. *Journal of Computational Chemistry*, 40(21):C1, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVv

[Ano19o] Anonymous. Cover image, volume 40, issue 22. *Journal of Computational Chemistry*, 40(22):C1, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVw

[Ano19p] Anonymous. Cover image, volume 40, issue 23. *Journal of Computational Chemistry*, 40(23):C1, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVx

[Ano19q] Anonymous. Cover image, volume 40, issue 24. *Journal of Computational Chemistry*, 40(24):C1, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVy

[Ano19r] Anonymous. Cover image, volume 40, issue 25. *Journal of Computational Chemistry*, 40(25):C1, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVz

[Ano19s] Anonymous. Cover image, volume 40, issue 26. *Journal of Computational Chemistry*, 40(26):C1, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVba

[Ano19t] Anonymous. Cover image, volume 40, issue 27. *Journal of Computational Chemistry*, 40(27):C1, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVbb

[Ano19u] Anonymous. Cover image, volume 40, issue 28. *Journal of Computational Chemistry*, 40(28):C1, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVbc

[Ano19v] Anonymous. Cover image, volume 40, issue 29. *Journal of Computational Chemistry*, 40(29):C1, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVc

[Ano19w] Anonymous. Cover image, volume 40, issue 3. *Journal of Computational Chemistry*, 40(3):C1, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVbd

[Ano19x] Anonymous. Cover image, volume 40, issue 30. *Journal of Computational Chemistry*, 40(30):C1, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVbe

[Ano19y] Anonymous. Cover image, volume 40, issue 31. *Journal of Computational Chemistry*, 40(31):C1, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVbf

[Ano19z] Anonymous. Cover image, volume 40, issue 32. *Journal of Computational Chemistry*, 40(32):C1, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVd

[Ano19-27] Anonymous. Cover image, volume 40, issue 4. *Journal of Computational Chemistry*, 40(4):C1, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVe

[Ano19-28] Anonymous. Cover image, volume 40, issue 5. *Journal of Computational Chemistry*, 40(5):C1, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVf

[Ano19-29] Anonymous. Cover image, volume 40, issue 6. *Journal of Computational Chemistry*, 40(6):C1, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVg

[Ano19-30] Anonymous. Cover image, volume 40, issue 7. *Journal of Computational Chemistry*, 40(7):C1, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVh

[Ano19-31] Anonymous. Cover image, volume 40, issue 8. *Journal of Computational Chemistry*, 40(8):C1, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:CIVi

[Ano19-32] Anonymous. Cover image, volume 40, issue 9. *Journal of Computational Chemistry*, 40(9):C1, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIa

[Ano19-33] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(1):1–10, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIb

[Ano19-34] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(2):288–296, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIc

[Ano19-35] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(3):549–553, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IId

[Ano19-36] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(4):625–629, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIe

[Ano19-37] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(5):707–711, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIf

[Ano19-38] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(6):763–767, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIg

[Ano19-39] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(7):849–853, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIh

[Ano19-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(8):911–915, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIi

[Ano19-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(9):959–964, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIj

[Ano19-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(10):1067–1072, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIk

[Ano19-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(11):1185–1189, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIl

[Ano19-44] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(12):1243–1247, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIm

[Ano19-45] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(13):1333–1337, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIn

[Ano19-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(14):1415–1419, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIo

[Ano19-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(15):1483–1487, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIp

[Ano19-48] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(16):1551–1555, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIq

[Ano19-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(17):1609–1613, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIr

[Ano19-50] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(18):1675–1679, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIs

[Ano19-51] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(19):1735, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIt

[Ano19-52] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(20):1801–1805, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIu

[Ano19-53] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(21):1875–1879, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIv

[Ano19-54] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(22):1931–1935, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIw

[Ano19-55] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(23):1995–1999, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIx

[Ano19-56] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(24):2067, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIy

[Ano19-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(25):2159–2163, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIz

[Ano19-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(26):2243–2247, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIba

[Ano19-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(27):2349–2353, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIbb

[Ano19-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(28):2439–2443, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIbc

[Ano19-61] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(29):2517–2521, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIbd

[Ano19-62] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(30):2597–2601, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIbe

[Ano19-63] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(31):2689–2693, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2019:IIbf

[Ano19-64] Anonymous. Issue information. *Journal of Computational Chemistry*, 40(32):2787–2792, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Antol:2013:PPN

[Ant13] Ivana Antol. Photodeactivation paths in norbornadiene. *Journal of Computational Chemistry*, 34(17):1439–1445, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anandakrishnan:2010:ABN

[AO10] Ramu Anandakrishnan and Alexey V. Onufriev. An $N \log N$ approximation based on the natural organization of biomolecules for speeding up the computation of long range interactions. *Journal of Computational Chemistry*, 31(4):691–706, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aoun:2016:FRB

[Aou16] Bachir Aoun. Fullrmc, a rigid body reverse Monte Carlo modeling package enabled with machine learning and artificial intelligence. *Journal of Computational Chemistry*, 37(12): 1102–1111, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akin-Ojo:2011:QBN

[AOW11] Omololu Akin-Ojo and Feng Wang. The quest for the best nonpolarizable water model from the adaptive force matching method. *Journal of Computational Chemistry*, 32(3):453–462, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arfeen:2014:ICC

[APA+14] Minhajul Arfeen, Dhilon S. Patel, Sheenu Abbat, Nikhil Taxak, and Prasad V. Bharatam. Importance of cytochromes in cyclization reactions: Quantum chemical study on a model reaction of proguanil to cycloguanil. *Journal of Computational Chemistry*, 35(28):2047–2055, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Allen:2014:SNU

[APK14] Bruce M. Allen, Paul K. Predecki, and Maciej Kumosa. Software news and updates: Integrating open-source software applications to build molecular dynamics systems. *Journal of Computational Chemistry*, 35(9):756–764, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arifin:2016:GTH

[APY+16] Arifin, Maneeporn Puripat, Daisuke Yokogawa, Vudhichai Parasuk, and Stephan Irle. Glucose transformation to 5-hydroxymethylfurfural in acidic ionic liquid: a quantum mechanical study. *Journal of Computational Chemistry*, 37(3): 327–335, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ali:2010:RCR

[AR10] Mohamad Akbar Ali and B. Rajakumar. Rate coefficients for the reaction of OH with $CF_3CH_2CH_3$ (HFC-263fb) between 200 and 400 K: ab initio, DFT, and transition state theory calculations. *Journal of Computational Chemistry*, 31(3):500–509, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anjos:2015:TAE

[AR15] Italo Curvelo Anjos and Gerd Bruno Rocha. A topological assessment of the electronic structure of mesoionic compounds. *Journal of Computational Chemistry*, 36(25):1907–1918, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anderson:2017:RSZ

[ARAG17] James S. M. Anderson, Juan I. Rodríguez, Paul W. Ayers, and Andreas W. Götz. Relativistic (SR-ZORA) quantum theory of atoms in molecules properties. *Journal of Computational Chemistry*, 38(2):81–86, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Avramopoulos:2013:VLN

[ARLP13] Aggelos Avramopoulos, Heribert Reis, Josep M. Luis, and Manthos G. Papadopoulos. On the vibrational linear and nonlinear optical properties of compounds involving noble gas atoms: HXeOXeH, HXeOXeF, and FXeOXeF. *Journal of Computational Chemistry*, 34(17):1446–1455, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alaniz:2015:AHI

[ARRC15] Víctor Duarte Alaniz, Tomás Rocha-Rinza, and Gabriel Cuevas. Assessment of hydrophobic interactions and their contributions through the analysis of the methane dimer. *Journal of Computational Chemistry*, 36(6):361–375, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aleksandrov:2010:MMM

[AS10] Alexey Aleksandrov and Thomas Simonson. A molecular mechanics model for imatinib and imatinib:kinase binding. *Journal of Computational Chemistry*, 31(7):1550–1560, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ajitha:2011:RSF

[AS11] Manjaly J. Ajitha and Cherumuttathu H. Suresh. Role of stereoelectronic features of imine and enamine in (S)-proline catalyzed Mannich reaction of acetaldehyde: an in silico study. *Journal of Computational Chemistry*, 32(9):1962–1970, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andersson:2014:PHE

[AS14] Martin P. Andersson and Susan L. S. Stipp. Predicting hydration energies for multivalent ions. *Journal of Computational Chemistry*, 35(28):2070–2075, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akbarzadeh:2015:HAA

[AS15a] Hamed Akbarzadeh and Amir Nasser Shamkhali. H_2 adsorption on Ag-nanocluster single-walled carbon nanotube composites: a molecular dynamics study on the effects of nanocluster size, diameter, and chirality of nanotube. *Journal of Computational Chemistry*, 36(7):433–440, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Antila:2015:CTI

[AS15b] Hanne S. Antila and Emppu Salonen. On combining Thole's induced point dipole model with fixed charge distributions in molecular mechanics force fields. *Journal of Computational Chemistry*, 36(10):739–750, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anjali:2018:PRP

[AS18] Bai Amutha Anjali and Cherumuttathu H. Suresh. Predicting reduction potentials of 1,3,6-triphenyl fulvenes using molecular electrostatic potential analysis of substituent effects. *Journal of Computational Chemistry*, 39(15):881–888, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Azadi:2018:NQE

[ASK18] Sam Azadi, Ranber Singh, and Thomas D. Kühne. Nuclear quantum effects induce metallization of dense solid molecular hydrogen. *Journal of Computational Chemistry*, 39(5):262–268, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alaghemandi:2011:CBT

[ASL$^+$11] Mohammad Alaghemandi, Joachim Schulte, Frédéric Leroy, Florian Müller-Plathe, and Michael C. Böhm. Correlation between thermal conductivity and bond length alternation in carbon nanotubes: a combined reverse nonequilibrium molecular dynamics — crystal orbital analysis. *Journal of Computational Chemistry*, 32(1):121–133, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ansbacher:2010:CDM

[ASMS10] Tamar Ansbacher, Hemant Kumar Srivastava, Jan M. L. Martin, and Avital Shurki. Can DFT methods correctly and efficiently predict the coordination number of copper(I) complexes? A case study. *Journal of Computational Chemistry*, 31(1):75–83, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Assadollahzadeh:2010:EPS

[ASS10] Behnam Assadollahzadeh, Sascha Schäfer, and Peter Schwerdtfeger. Electronic properties for small tin clusters Sn_n

($n \leq 20$) from density functional theory and the convergence toward the solid state. *Journal of Computational Chemistry*, 31(5):929–937, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Amaouch:2017:BPH

[ASS+17] Mohamed Amaouch, Dumitru-Claudiu Sergentu, David Steinmetz, Rémi Maurice, Nicolas Galland, and Julien Pilmé. The bonding picture in hypervalent XF_3 (X = Cl, Br, I, At) fluorides revisited with quantum chemical topology. *Journal of Computational Chemistry*, 38(32):2753–2762, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abramyan:2016:CAM

[AST+16] Tigran M. Abramyan, James A. Snyder, Aby A. Thyparambil, Steven J. Stuart, and Robert A. Latour. Cluster analysis of molecular simulation trajectories for systems where both conformation and orientation of the sampled states are important. *Journal of Computational Chemistry*, 37(21):1973–1982, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ang:2019:MHB

[ASW19] Shi Jun Ang, Cher Tian Ser, and Ming Wah Wong. Modeling halogen bonding with planewave density functional theory: Accuracy and challenges. *Journal of Computational Chemistry*, 40(20):1829–1835, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alvarez-Thon:2018:SOE

[ATIP18] Luis Alvarez-Thon and Natalia Inostroza-Pino. Spin-orbit effects on magnetically induced current densities in the M_5^- clusters (M = N, P, As, Sb, Bi, Mc). *Journal of Computational Chemistry*, 39(14):862–868, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alvarez-Thon:2018:IGP

[ATM18] Luis Alvarez-Thon and Liliana Mammino. Information on gas-phase diatomic molecules from magnetically induced current densities. *Journal of Computational Chemistry*, 39(1):52–60, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alkorta:2018:IQA

[ATP18] Ibon Alkorta, Joseph C. R. Thacker, and Paul L. A. Popelier. An interacting quantum atom study of model S_N2 reactions (X^- ···CH_3 X, X = F, Cl, Br, and I). *Journal of Computational Chemistry*, 39(10):546–556, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Avdoshenko:2018:FFC

[Avd18] Stanislav M. Avdoshenko. Fullerene Faraday cage keeps magnetic properties of inner cluster pristine. *Journal of Computational Chemistry*, 39(21):1594–1598, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Acke:2018:IBN

[AVHB18] Guillaume Acke, Sofie Van Damme, Remco W. A. Havenith, and Patrick Bultinck. Interpreting the behavior of the NICSzz by resolving in orbitals, sign, and positions. *Journal of Computational Chemistry*, 39(9):511–519, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Achazi:2016:TEI

[AvKSP16] Andreas J. Achazi, Larissa K. S. von Krbek, Christoph A. Schalley, and Beate Paulus. Theoretical and experimental investigation of crown/ammonium complexes in solution. *Journal of Computational Chemistry*, 37(1):18–24, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

An:2018:TIC

[AWF+18] Beibei An, Keke Wen, Songyan Feng, Xiao Pan, Wenpeng Wu, Xugeng Guo, and Jinglai Zhang. Theoretical insights into the 1D-charge transport properties in a series of hexaazatrinaphthylene-based discotic molecules. *Journal of Computational Chemistry*, 39(13):773–779, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andoh:2017:EAP

[AYYO17] Yoshimichi Andoh, Noriyuki Yoshii, Atsushi Yamada, and Susumu Okazaki. Evaluation of atomic pressure in the multiple time-step integration algorithm. *Journal of Computa-*

tional Chemistry, 38(10):704–713, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burger:2011:EPP

[BA11] Steven K. Burger and Paul W. Ayers. Empirical prediction of protein pK_a values with residue mutation. *Journal of Computational Chemistry*, 32(10):2140–2148, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bachler:2012:QCC

[Bac12] Vinzenz Bachler. A quantum chemical calculation on $Fe(CO)_5$ revealing the operation of the Dewar–Chatt–Duncanson model. *Journal of Computational Chemistry*, 33(24):1936–1947, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borras-Almenar:2010:MPC

[BACSCJ+10] J. J. Borrás-Almenar, S. Cardona-Serra, J. M. Clemente-Juan, E. Coronado, A. V. Palii, and B. S. Tsukerblat. MV-PACK: a package to calculate energy levels and magnetic properties of high nuclearity mixed valence clusters. *Journal of Computational Chemistry*, 31(6):1321–1332, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhagat:2019:ELP

[BAD+19] Shweta Bhagat, Minhajul Arfeen, Gourav Das, Neha Patel, and Prasad V. Bharatam. Electronic and ligating properties of carbocyclic carbenes: a theoretical investigation. *Journal of Computational Chemistry*, 40(5):726–733, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beu:2018:CFF

[BAF18] Titus Adrian Beu, Andrada-Elena Ailenei, and Alexandra Farcas. CHARMM force field for protonated polyethyleneimine. *Journal of Computational Chemistry*, 39(31):2564–2575, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balius:2013:GBM

[BAMR13] Trent E. Balius, William J. Allen, Sudipto Mukherjee, and Robert C. Rizzo. Grid-based molecular footprint comparison method for docking and de novo design: Application to HIVgp41. *Journal of Computational Chemistry*, 34(14):1226–1240, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranov:2014:ELI

[Bar14] Alexey I. Baranov. Electron localizability indicators from spinor wavefunctions. *Journal of Computational Chemistry*, 35(7):565–585, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burger:2014:EPT

[BAS14] Steven K. Burger, Paul W. Ayers, and Jeremy Schofield. Efficient parameterization of torsional terms for force fields. *Journal of Computational Chemistry*, 35(19):1438–1445, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boresch:2011:AVW

[BB11a] Stefan Boresch and Stefan Bruckner. Avoiding the van der Waals endpoint problem using serial atomic insertion. *Journal of Computational Chemistry*, 32(11):2449–2458, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruckner:2011:EAFa

[BB11b] Stefan Bruckner and Stefan Boresch. Efficiency of alchemical free energy simulations. I. A practical comparison of the exponential formula, thermodynamic integration, and Bennett's acceptance ratio method. *Journal of Computational Chemistry*, 32(7):1303–1319, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruckner:2011:EAFb

[BB11c] Stefan Bruckner and Stefan Boresch. Efficiency of alchemical free energy simulations. II. Improvements for thermodynamic integration. *Journal of Computational Chemistry*, 32(7):1320–1333, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bachorz:2011:MFM

[BBG+11] Rafał A. Bachorz, Florian A. Bischoff, Andreas Glöß, Christof Hättig, Sebastian Höfener, Wim Klopper, and David P. Tew.

The MP2-F12 method in the T URBOMOLE program package. *Journal of Computational Chemistry*, 32(11):2492–2513, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Banerjee:2018:CPS

[BBG+18a] Jaita Banerjee, Stefan Behnle, Martin C. E. Galbraith, Volker Settels, Bernd Engels, Ralf Tonner, and Reinhold F. Fink. Comparison of the periodic slab approach with the finite cluster description of metal-organic interfaces at the example of PTCDA on Ag(110). *Journal of Computational Chemistry*, 39 (14):844–852, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bronova:2018:SNU

[BBG+18b] Anna Bronova, Thomas Bredow, Robert Glaum, Mark J. Riley, and Werner Urland. Software news and updates: BonnMag: Computer program for ligand-field analysis of f^n systems within the angular overlap model. *Journal of Computational Chemistry*, 39(3):176–186, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bucinsky:2011:REH

[BBI+11] Lukáš Bučinský, Stanislav Biskupič, Michal Ilčin, Vladimír Lukeš, and Viliam Laurinc. Relativistic effects in HgHe and HgXe CCSD(T) ground state potential curves. Low-density viscosity simulations of Hg:Xe mixture. *Journal of Computational Chemistry*, 32(2):356–367, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bazgier:2016:ERI

[BBOB16] Václav Bazgier, Karel Berka, Michal Otyepka, and Pavel Banáš. Exponential repulsion improves structural predictability of molecular docking. *Journal of Computational Chemistry*, 37(28):2485–2494, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burger:2013:EOV

[BC13] Steven K. Burger and G. Andrés Cisneros. Efficient optimization of van der Waals parameters from bulk properties. *Journal of Computational Chemistry*, 34(27):2313–2319, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bond:2010:FOS

[BCCO10] Stephen D. Bond, Jehanzeb Hameed Chaudhry, Eric C. Cyr, and Luke N. Olson. A first-order system least-squares finite element method for the Poisson–Boltzmann equation. *Journal of Computational Chemistry*, 31(8):1625–1635, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borrelli:2010:EHR

[BCG10] Kenneth W. Borrelli, Benjamin Cossins, and Victor Guallar. Exploring hierarchical refinement techniques for induced fit docking with protein and ligand flexibility. *Journal of Computational Chemistry*, 31(6):1224–1235, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baldovi:2014:LEU

[BCJC+14] José J. Baldoví, Juan M. Clemente-Juan, Eugenio Coronado, Alejandro Gaita-Ariño, and Andrew Palii. Letters to the Editor: An updated version of the computational package SIMPRE that uses the standard conventions for Stevens crystal field parameters. *Journal of Computational Chemistry*, 35 (26):1930–1934, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bartolomei:2011:LRI

[BCNH+11] Massimiliano Bartolomei, Estela Carmona-Novillo, Marta I. Hernández, José Campos-Martínez, and Ramón Hernández-Lamoneda. Long-range interaction for dimers of atmospheric interest: dispersion, induction and electrostatic contributions for O_2O_2, N_2N_2 and O_2N_2. *Journal of Computational Chemistry*, 32(2):279–290, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borghini:2010:CRP

[BCP+10] Alice Borghini, Paolo Crotti, Daniele Pietra, Lucilla Favero, and Anna Maria Bianucci. Chemical reactivity predictions: Use of data mining techniques for analyzing regioselective azidolysis of epoxides. *Journal of Computational Chemistry*, 31(14):2612–2619, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baldovi:2013:SNU

[BCSCJ+13] José J. Baldoví, Salvador Cardona-Serra, Juan M. Clemente-Juan, Eugenio Coronado, Alejandro Gaita-Ariño, and Andrew Palii. Software news and updates: SIMPRE: a software package to calculate crystal field parameters, energy levels, and magnetic properties on mononuclear lanthanoid complexes based on charge distributions. *Journal of Computational Chemistry*, 34(22):1961–1967, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brice:2011:ARM

[BD11] Allyn R. Brice and Brian N. Dominy. Analyzing the robustness of the MM/PBSA free energy calculation method: Application to DNA conformational transitions. *Journal of Computational Chemistry*, 32(7):1431–1440, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boschitsch:2012:FNS

[BD12] Alexander H. Boschitsch and Pavel V. Danilov. Formulation of a new and simple nonuniform size-modified Poisson–Boltzmann description. *Journal of Computational Chemistry*, 33(11):1152–1164, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brasil:2013:MEA

[BDdS13] Christiane Regina Soares Brasil, Alexandre Claudio Botazzo Delbem, and Fernando Luís Barroso da Silva. Multiobjective evolutionary algorithm with many tables for purely ab initio protein structure prediction. *Journal of Computational Chemistry*, 34(20):1719–1734, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bauer:2011:MDS

[BDTP11] Brad A. Bauer, Joseph E. Davis, Michela Taufer, and Sandeep Patel. Molecular dynamics simulations of aqueous ions at the liquid–vapor interface accelerated using graphics processors. *Journal of Computational Chemistry*, 32(3):375–385, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandura:2012:FPC

[BE12] Andrei V. Bandura and Robert A. Evarestov. First-principles calculations on thermodynamic properties of $BaTiO_3$ rhombohedral phase. *Journal of Computational Chemistry*, 33(18): 1554–1563, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandura:2014:TZS

[BE14] Andrei V. Bandura and Robert A. Evarestov. TiS_2 and ZrS_2 single- and double-wall nanotubes: First-principles study. *Journal of Computational Chemistry*, 35(5):395–405, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruckner:2016:TDC

[BE16] Charlotte Brückner and Bernd Engels. A theoretical description of charge reorganization energies in molecular organic P-type semiconductors. *Journal of Computational Chemistry*, 37(15):1335–1344, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bendazzoli:2014:TPS

[BEEL14] Gian Luigi Bendazzoli, Muammar El Khatib, Stefano Evangelisti, and Thierry Leininger. The total Position Spread in mixed-valence compounds: a study on the H4+ model system. *Journal of Computational Chemistry*, 35(10):802–808, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brooks:2013:ENP

[BEFS13] Charles L. Brooks III, Masahiro Ehara, Gernot Frenking, and Peter R. Schreiner. Editorials: New paint and a new engine. *Journal of Computational Chemistry*, 34(1):1, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bushnell:2011:FBP

[BEL+11] Eric A. C. Bushnell, Edvin Erdtman, Jorge Llano, Leif A. Eriksson, and James W. Gauld. The first branching point in porphyrin biosynthesis: a systematic docking, molecular dynamics and quantum mechanical/molecular mechanical study of substrate binding and mechanism of uroporphyrinogen-III decarboxylase. *Journal of Computational Chemistry*, 32(5): 822–834, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandaru:2014:IES

[BEM14] Sateesh Bandaru, Niall J. English, and J. M. D. MacElroy. Implicit and explicit solvent models for modeling a bifunctional arene ruthenium hydrogen-storage catalyst: a classical and ab initio molecular simulation study. *Journal of Computational Chemistry*, 35(9):683–691, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benassi:2017:BDF

[Ben17] Enrico Benassi. Benchmarking of density functionals for a soft but accurate prediction and assignment of ^{1}H and ^{13}C NMR chemical shifts in organic and biological molecules. *Journal of Computational Chemistry*, 38(2):87–92, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandaru:2014:TDN

[BEPM14] Sateesh Bandaru, Niall J. English, Andrew D. Phillips, and J. M. D. MacElroy. Towards the design of novel boron- and nitrogen-substituted ammonia-borane and bifunctional arene ruthenium catalysts for hydrogen storage. *Journal of Computational Chemistry*, 35(12):891–903, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bernardes:2017:SNU

[Ber17] Carlos E. S. Bernardes. Software news and updates: AGGREGATES: Finding structures in simulation results of solutions. *Journal of Computational Chemistry*, 38(10):753–765, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barigye:2015:MAI

[BF15] Stephen J. Barigye and Matheus P. Freitas. Is molecular alignment an indispensable requirement in the MIA-QSAR method? *Journal of Computational Chemistry*, 36(23):1748–1755, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beu:2017:CFF

[BF17] Titus Adrian Beu and Alexandra Farcaş. CHARMM force field and molecular dynamics simulations of protonated polyethylenimine. *Journal of Computational Chemistry*, 38 (27):2335–2348, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Batlogg:2019:CAM

[BF19a] Aymerick Batlogg and Maria Fumanal. Computational assessment of MLCT versus MC stabilities in first-to-third-row d^6 pseudo-octahedral transition metal complexes. *Journal of Computational Chemistry*, 40(27):2377–2390, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bernales:2019:RCH

[BF19b] Varinia Bernales and Robert D. Froese. Rhodium catalyzed hydroformylation of olefins. *Journal of Computational Chemistry*, 40(2):342–348, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boomsma:2013:SNU

[BFH+13] Wouter Boomsma, Jes Frellsen, Tim Harder, Sandro Bottaro, Kristoffer E. Johansson, Pengfei Tian, Kasper Støvgaard, Christian Andreetta, Simon Olsson, Jan B. Valentin, Lubomir D. Antonov, Anders S. Christensen, Mikael Borg, Jan H. Jensen, Kresten Lindorff-Larsen, Jesper Ferkinghoff-Borg, and Thomas Hamelryck. Software news and updates: PHAISTOS: a framework for Markov chain Monte Carlo simulation and inference of protein structure. *Journal of Computational Chemistry*, 34(19):1697–1705, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buelens:2012:LSS

[BG12] Floris P. Buelens and Helmut Grubmüller. Linear-scaling soft-core scheme for alchemical free energy calculations. *Journal of Computational Chemistry*, 33(1):25–33, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bushnell:2013:APH

[BG13] Eric A. C. Bushnell and James W. Gauld. An assessment of pure, hybrid, meta, and hybrid-meta GGA density functional theory methods for open-shell systems: the case of the nonheme iron enzyme 8R–LOX. *Journal of Computational Chemistry*, 34(2):141–148, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bose:2017:IED

[BG17] Samik Bose and Debashree Ghosh. An interaction energy driven biased sampling technique: a faster route to ionization spectra in condensed phase. *Journal of Computational Chemistry*, 38(26):2248–2257, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhatia:2018:TMC

[BGL+18] Harsh Bhatia, Attila G. Gyulassy, Vincenzo Lordi, John E. Pask, Valerio Pascucci, and Peer-Timo Bremer. Topo MS: Comprehensive topological exploration for molecular and condensed-matter systems. *Journal of Computational Chemistry*, 39(16):936–952, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bosson:2013:BAQ

[BGR13] Maël Bosson, Sergei Grudinin, and Stephane Redon. Block-adaptive quantum mechanics: an adaptive divide-and-conquer approach to interactive quantum chemistry. *Journal of Computational Chemistry*, 34(6):492–504, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borocci:2019:NCN

[BGS+19] Stefano Borocci, Felice Grandinetti, Nico Sanna, Paola Antoniotti, and Francesca Nunzi. Noncovalent complexes of the noble-gas atoms: Analyzing the transition from physical to chemical interactions. *Journal of Computational Chemistry*, 40(26):2318–2328, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brovarets:2013:AUC

[BH13] Ol'ha O. Brovarets' and Dmytro M. Hovorun. Atomistic understanding of the C·T mismatched DNA base pair tautomerization via the DPT: QM and QTAIM computational approaches. *Journal of Computational Chemistry*, 34(30): 2577–2590, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berco:2014:SHT

[BH14] Dan Berco and Chin-Kun Hu. A spherical harmonic transform spectral analysis of a localized surface plasmon on a gold nano shell. *Journal of Computational Chemistry*, 35(30): 2225–2230, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See corrigendum [Ano15-58].

Bieler:2015:OSF

[BH15] Noah S. Bieler and Philippe H. Hünenberger. Orthogonal sampling in free-energy calculations of residue mutations in a tripeptide: TI versus λ-LEUS. *Journal of Computational Chemistry*, 36(22):1686–1697, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

BenAmor:2019:RSV

[BH19] Nadia Ben Amor and Marie-Catherine Heitz. RASPT2 study of the valence excited states of an iron-porphyrin-carbonyl model complex. *Journal of Computational Chemistry*, 40(17): 1614–1621, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balabin:2012:SNU

[BHB12] Ilya A. Balabin, Xiangqian Hu, and David N. Beratan. Software news and updates: Exploring biological electron transfer pathway dynamics with the Pathways Plugin for VMD. *Journal of Computational Chemistry*, 33(8):906–910, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Belzunces:2017:TSA

[BHB+17] Bastien Belzunces, Sophie Hoyau, Magali Benoit, Nathalie Tarrat, and Fabienne Bessac. Theoretical study of the atrazine pesticide interaction with pyrophyllite and Ca^{2+}-montmorillonite clay surfaces. *Journal of Computational Chemistry*, 38(3):133–143, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Belzunces:2019:IMF

[BHB19] Bastien Belzunces, Sophie Hoyau, and Fabienne Bessac. Interaction of Metamitron and Fenhexamid with Ca^{2+}-montmorillonite clay surfaces: a density functional theory molecular dynamics study. *Journal of Computational Chemistry*, 40(14):1449–1462, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barletta:2018:DFA

[BHF+18] German P. Barletta, Marcia Anahi Hasenahuer, Maria Silvina Fornasari, Gustavo Parisi, and Sebastian Fernandez-Alberti. Dynamics fingerprints of active conformers of epidermal growth factor receptor kinase. *Journal of Computational Chemistry*, 39(29):2472–2480, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baltoumas:2019:GNO

[BHI19] Fotis A. Baltoumas, Stavros J. Hamodrakas, and Vassiliki A. Iconomidou. The gram-negative outer membrane modeler: Automated building of lipopolysaccharide-rich bacterial outer membranes in four force fields. *Journal of Computational Chemistry*, 40(18):1727–1734, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baba:2014:IFM

[BHNS14] Takeshi Baba, Ryuhei Harada, Masayoshi Nakano, and Yasuteru Shigeta. On the induced-fit mechanism of substrate-enzyme binding structures of nylon-oligomer hydrolase. *Journal of Computational Chemistry*, 35(16):1240–1247, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Batool:2019:MSH

[BHP19] Javaria Batool, Torsten Hahn, and Mark R. Pederson. Magnetic signatures of hydroxyl- and water-terminated neutral and tetra-anionic Mn_12-acetate. *Journal of Computational Chemistry*, 40(26):2301–2308, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bergeler:2015:MTB

[BHR15] Maike Bergeler, Carmen Herrmann, and Markus Reiher. Mode-tracking based stationary-point optimization. *Jour-*

nal of Computational Chemistry, 36(19):1429–1438, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boo:2010:IDS

[BIL10] Bong Hyun Boo, Suk Im, and Sungyul Lee. Ab initio and DFT studies of the thermal rearrangement of trimethylsilyl(methyl)silylene: Remarkable rearrangements of silicon intermediates. *Journal of Computational Chemistry*, 31(1):154–163, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bevc:2015:SNU

[BJP15] Staš Bevc, Christoph Junghans, and Matej Praprotnik. Software news and updates: STOCK: Structure mapper and online coarse-graining kit for molecular simulations. *Journal of Computational Chemistry*, 36(7):467–477, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berezniak:2012:SDA

[BJSI12] Tomasz Bereźniak, Andres Jäschke, Jeremy C. Smith, and Petra Imhof. Stereoselection in the Diels–Alderase ribozyme: a molecular dynamics study. *Journal of Computational Chemistry*, 33(19):1603–1614, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranov:2011:ELD

[BK11] Alexey I. Baranov and Miroslav Kohout. Electron localization and delocalization indices for solids. *Journal of Computational Chemistry*, 32(10):2064–2076, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boateng:2013:CTC

[BK13] Henry A. Boateng and Robert Krasny. Comparison of treecodes for computing electrostatic potentials in charged particle systems with disjoint targets and sources. *Journal of Computational Chemistry*, 34(25):2159–2167, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Banushkina:2015:FSA

[BK15] Polina V. Banushkina and Sergei V. Krivov. Fep1d: a script for the analysis of reaction coordinates. *Journal of Computational Chemistry*, 36(12):878–882, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bazzoli:2017:SHB

[BK17a] Andrea Bazzoli and John Karanicolas. "Solvent hydrogen-bond occlusion": a new model of polar desolvation for biomolecular energetics. *Journal of Computational Chemistry*, 38(16):1321–1331, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borpuzari:2017:NNT

[BK17b] Manash Protim Borpuzari and Rahul Kar. A new nonempirical tuning scheme with single self-consistent field calculation: Comparison with global and IP-tuned range-separated functional. *Journal of Computational Chemistry*, 38(26):2258–2267, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bykov:2017:GED

[BK17c] Dmytro Bykov and Thomas Kjaergaard. The GPU-enabled divide-expand-consolidate RI-MP2 method (DEC-RI-MP2). *Journal of Computational Chemistry*, 38(4):228–237, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bilbrey:2013:ELC

[BKLA13] Jenna A. Bilbrey, Arianna H. Kazez, Jason Locklin, and Wesley D. Allen. Exact ligand cone angles. *Journal of Computational Chemistry*, 34(14):1189–1197, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baldes:2011:ASC

[BKŠ+11] Alexander Baldes, Wim Klopper, Ján Šimunek, Jozef Noga, and Florian Weigend. Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure. *Journal of Computational Chemistry*, 32(14):3129–3134, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buenker:2012:ISP

[BL12] Robert J. Buenker and Heinz-Peter Liebermann. Ab initio study of the positronation of the CaO and SrO molecules including calculation of annihilation rates. *Journal of Computational Chemistry*, 33(19):1594–1602, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barquera-Lozada:2019:VSA

[BL19] José E. Barquera-Lozada. Vorticity: Simplifying the analysis of the current density. *Journal of Computational Chemistry*, 40(30):2602–2610, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska-Laczkowska:2013:PLR

[BŁBG+13] Angelika Baranowska-Łaczkowska, Wojciech Bartkowiak, Robert W. Góra, Filip Pawłowski, and Robert Zaleśny. On the performance of long-range-corrected density functional theory and reduced-size polarized LPol-n basis sets in computations of electric dipole (hyper)polarizabilities of π-conjugated molecules. *Journal of Computational Chemistry*, 34(10):819–826, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beker:2013:LCP

[BLDK+13] Wiktor Beker, Karol M. Langner, Edyta Dyguda-Kazimierowicz, Mikołaj Feliks, and W. Andrzej Sokalski. Low cost prediction of relative stabilities of hydrogen bonded complexes from atomic multipole moments for overly short intermolecular distances. *Journal of Computational Chemistry*, 34(21):1797–1799, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska-Laczkowska:2014:BSE

[BŁF14] Angelika Baranowska-Łaczkowska and Berta Fernández. Basis sets for the evaluation of van der Waals complex interaction energies: Ne–N_2 intermolecular potential and microwave spectrum. *Journal of Computational Chemistry*, 35(3):199–203, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska-Laczkowska:2013:NBS

[BŁFZ13] Angelika Baranowska-Łaczkowska, Berta Fernández, and Robert Zaleśny. New basis sets for the evaluation of interaction-induced electric properties in hydrogen-bonded complexes. *Journal of Computational Chemistry*, 34(4):275–283, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berski:2010:IQC

[BLG10] Slawomir Berski, Zdzislaw Latajka, and Agnieszka J. Gordon. Ab initio and Quantum Chemical Topology studies on the isomerization of HONO to HNO_2. Effect of the basis set in QCT. *Journal of Computational Chemistry*, 31(14):2555–2567, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berski:2011:ELF

[BLG11] Slawomir Berski, Zdzislaw Latajka, and Agnieszka J. Gordon. Electron localization function and electron localizability indicator applied to study the bonding in the peroxynitrous acid HOONO. *Journal of Computational Chemistry*, 32(8):1528–1540, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bezkorovaynaya:2012:MSS

[BLKP12] Olga Bezkorovaynaya, Alexander Lukyanov, Kurt Kremer, and Christine Peter. Multiscale simulation of small peptides: Consistent conformational sampling in atomistic and coarse-grained models. *Journal of Computational Chemistry*, 33(9):937–949, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska-Laczkowska:2013:OBS

[BŁŁ13] Angelika Baranowska-Łaczkowska and Krzysztof Z. Łaczkowski. The ORP basis set designed for optical rotation calculations. *Journal of Computational Chemistry*, 34(23):2006–2013, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska:2010:MSO

[BŁS10] Angelika Baranowska, Krzysztof Z. Łaczkowski, and Andrzej J. Sadlej. Model studies of the optical rotation, and theoretical determination of its sign for β-pinene and *trans*-pinane. *Journal of Computational Chemistry*, 31(6):1176–1181, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buenker:2013:ABO

[BLZ+13] Robert J. Buenker, Heinz-Peter Liebermann, Yu Zhang, Yong Wu, Lingling Yan, Chunhua Liu, Yizhi Qu, and Jianguo Wang. Adjustment of Born–Oppenheimer electronic wave functions to simplify close coupling calculations. *Journal of Computational Chemistry*, 34(11):928–937, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barbault:2012:IPB

[BM12] Florent Barbault and François Maurel. Is inhibition process better described with MD(QM/MM) simulations? The case of urokinase type plasminogen activator inhibitors. *Journal of Computational Chemistry*, 33(6):607–616, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhatia:2013:EDT

[BMB13] Sonam Bhatia, Yogesh J. Malkhede, and Prasad V. Bharatam. Existence of dynamic tautomerism and divalent N(I) character in N-(pyridin-2-yl)thiazol-2-amine. *Journal of Computational Chemistry*, 34(18):1577–1588, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borstnik:2011:DDF

[BMBJ11] Urban Borštnik, Benjamin T. Miller, Bernard R. Brooks, and Dušanka Janežič. The distributed diagonal force decomposition method for parallelizing molecular dynamics simulations. *Journal of Computational Chemistry*, 32(14):3005–3013, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhattacharjee:2019:APJ

[BMD19] Rameswar Bhattacharjee, Tirthick Majumder, and Ayan Datta. Analysis of pseudo Jahn–Teller distortion based on natural bond orbital theory: Case study for silicene. *Journal of Computational Chemistry*, 40(15):1488–1495, June 5,

2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Branduardi:2016:ARD

[BMFG16] Davide Branduardi, Fabrizio Marinelli, and José D. Faraldo-Gómez. Atomic-resolution dissection of the energetics and mechanism of isomerization of hydrated ATP-Mg^{2+} through the SOMA string method. *Journal of Computational Chemistry*, 37(6):575–586, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barigye:2013:RFH

[BMPML+13] Stephen J. Barigye, Yovani Marrero-Ponce, Yoan Martínez-López, Francisco Torrens, Luis Manuel Artiles-Martínez, Ricardo W. Pino-Urias, and Oscar Martínez-Santiago. Relations frequency hypermatrices in mutual, conditional and joint entropy-based information indices. *Journal of Computational Chemistry*, 34(4):259–274, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balius:2011:IED

[BMR11] Trent E. Balius, Sudipto Mukherjee, and Robert C. Rizzo. Implementation and evaluation of a docking-rescoring method using molecular footprint comparisons. *Journal of Computational Chemistry*, 32(10):2273–2289, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boulougouris:2014:FEC

[Bou14] Georgios C. Boulougouris. Free energy calculations, enhanced by a Gaussian ansatz, for the “chemical work” distribution. *Journal of Computational Chemistry*, 35(13):1024–1035, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bowman:2016:AMN

[Bow16] Gregory R. Bowman. Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. *Journal of Computational Chemistry*, 37(6):558–566, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bozkaya:2018:AEG

[Boz18] Uğur Bozkaya. Analytic energy gradients for orbital-optimized MP3 and MP2.5 with the density-fitting approximation: an efficient implementation. *Journal of Computational Chemistry*, 39(7):351–360, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bohme:2018:RDM

[BP18] Michael Böhme and Winfried Plass. rhOver: Determination of magnetic anisotropy and related properties for dysprosium(III) single-ion magnets by semiempirical approaches utilizing Hartree–Fock wave functions. *Journal of Computational Chemistry*, 39(32):2697–2712, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bordogna:2011:PAP

[BPB11] Annalisa Bordogna, Alessandro Pandini, and Laura Bonati. Predicting the accuracy of protein–ligand docking on homology models. *Journal of Computational Chemistry*, 32(1):81–98, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borkar:2013:HBC

[BPC13] Mahesh R. Borkar, Raghuvir R. S. Pissurlenkar, and Evans C. Coutinho. HomoSAR: Bridging comparative protein modeling with quantitative structural activity relationship to design new peptides. *Journal of Computational Chemistry*, 34(30):2635–2646, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beata:2019:CNT

[BPC19] Giorgia Beata, Gianpaolo Perego, and Bartolomeo Civalleri. CRYSPLOT: a new tool to visualize physical and chemical properties of molecules, polymers, surfaces, and crystalline solids. *Journal of Computational Chemistry*, 40(26):2329–2338, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandura:2016:AZF

[BPE16] Andrei V. Bandura, Vitaly V. Porsev, and Robert A. Evarestov. Application of zone-folding approach to the first-principles estimation of thermodynamic properties of carbon and ZrS_2-based nanotubes. *Journal of Computational Chemistry*, 37(7):641–652, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bartolomei:2012:FDG

[BPLL12] Massimiliano Bartolomei, Fernando Pirani, Antonio Laganà, and Andrea Lombardi. A full dimensional grid empowered simulation of the $CO_2 + CO_2$ processes. *Journal of Computational Chemistry*, 33(22):1806–1819, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bartolomei:2015:LES

[BPM15] M. Bartolomei, F. Pirani, and J. M. C. Marques. Low-energy structures of benzene clusters with a novel accurate potential surface. *Journal of Computational Chemistry*, 36(31):2291–2301, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandara:2017:ESS

[BPPS17] Asanga Bandara, Afra Panahi, George A. Pantelopulos, and John E. Straub. Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers. *Journal of Computational Chemistry*, 38(16):1479–1488, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandara:2019:ESS

[BPPS19] Asanga Bandara, Afra Panahi, George A. Pantelopulos, and John E. Straub. Exploring the structure and stability of cholesterol dimer formation in multicomponent lipid bilayers. *Journal of Computational Chemistry*, 40(26):2348, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bello-Rivas:2016:STK

[BRE16] Juan M. Bello-Rivas and Ron Elber. Simulations of thermodynamics and kinetics on rough energy landscapes with milestoning. *Journal of Computational Chemistry*, 37(6):602–613, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beheshti:2012:HTO

[BRGN12] Abolghasem Beheshti, Siavash Riahi, Mohammad Reza Ganjali, and Parviz Norouzi. Highlighting and trying to overcome a serious drawback with QSPR studies; data collection in different experimental conditions (mixed-QSPR). *Journal of Computational Chemistry*, 33(7):732–747, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bondesson:2008:BSD

[BRLS08] Laban Bondesson, Elias Rudberg, Yi Luo, and Paweł Sałek. Basis set dependence of solute–solvent interaction energy of benzene in water: a HF/DFT study. *Journal of Computational Chemistry*, 29(11):1725–1732, August 2008. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [BRLS12].

Bondesson:2012:EBS

[BRLS12] Laban Bondesson, Elias Rudberg, Yi Luo, and Paweł Sałek. Erratum: "Basis set dependence of solute–solvent interaction energy of benzene in water: a HF/DFT study". *Journal of Computational Chemistry*, 33(3):354, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [BRLS08].

Bosson:2012:IQC

[BRP+12] Mäel Bosson, Caroline Richard, Antoine Plet, Sergei Grudinin, and Stephane Redon. Interactive quantum chemistry: a divide-and-conquer ASED-MO method. *Journal of Computational Chemistry*, 33(7):779–790, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baranowska:2010:PBS

[BS10a] Angelika Baranowska and Andrzej J. Sadlej. Polarized basis sets for accurate calculations of static and dynamic electric properties of molecules. *Journal of Computational Chemistry*, 31(3):552–560, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Black:2010:BHH

[BS10b] Gráinne Black and John M. Simmie. Barrier heights for H-atom abstraction by $\dot{H}O_2$ from *n*-butanol — a simple yet ex-acting test for model chemistries? *Journal of Computational Chemistry*, 31(6):1236–1248, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brylinski:2010:QDL

[BS10c] Michal Brylinski and Jeffrey Skolnick. Q-Dock^{LHM}: Low-resolution refinement for ligand comparative modeling. *Journal of Computational Chemistry*, 31(5):1093–1105, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Birkholz:2015:UBG

[BS15] Adam B. Birkholz and H. Bernhard Schlegel. Using bonding to guide transition state optimization. *Journal of Computational Chemistry*, 36(15):1157–1166, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Blomberg:2016:IFE

[BS16a] Margareta R. A. Blomberg and Per E. M. Siegbahn. Improved free energy profile for reduction of NO in cytochrome c dependent nitric oxide reductase (cNOR). *Journal of Computational Chemistry*, 37(19):1810–1818, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boese:2016:AAE

[BS16b] A. Daniel Boese and Joachim Sauer. Accurate adsorption energies for small molecules on oxide surfaces: CH_4 /MgO(001) and C_2H_6 /MgO(001). *Journal of Computational Chemistry*, 37(26):2374–2385, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buchholz:2018:ALE

[BS18] Hannes Konrad Buchholz and Matthias Stein. Accurate lattice energies of organic molecular crystals from periodic Turbomole calculations. *Journal of Computational Chemistry*, 39(19):1335–1343, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Becker:2019:DFT

[BS19] Martin Becker and Marek Sierka. Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Stress tensor. *Journal* of *Computational Chemistry*, 40(29):2563–2570, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bejagam:2018:DNB

[BSD18] Karteek K. Bejagam, Samrendra Singh, and Sanket A. Deshmukh. Development of non-bonded interaction parameters between graphene and water using particle swarm optimization. *Journal of Computational Chemistry*, 39(12):721–734, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borthakur:2016:TST

[BSDP16] Bitupon Borthakur, Bernard Silvi, Rian D. Dewhurst, and Ashwini K. Phukan. Theoretical strategies toward stabilization of singlet remote N-heterocyclic carbenes. *Journal of Computational Chemistry*, 37(16):1484–1490, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bauza:2018:MEP

[BSF18] Antonio Bauzá, Saikat Kumar Seth, and Antonio Frontera. Molecular electrostatic potential and "atoms-in-molecules" analyses of the interplay between π-hole and lone pair$\cdots\pi$ / X–H$\cdots\pi$ /metal$\cdots\pi$ interactions. *Journal of Computational Chemistry*, 39(9):458–463, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bijina:2018:EPL

[BSG18a] Padinjare Veetil Bijina, Cherumuttathu H. Suresh, and Shridhar R. Gadre. Electrostatics for probing lone pairs and their interactions. *Journal of Computational Chemistry*, 39(9):488–499, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bukharov:2018:HCI

[BSG$^+$18b] Mikhail S. Bukharov, Valery G. Shtyrlin, Edward M. Gilyazetdinov, Nikita Yu. Serov, and Timur I. Madzhidov. Hydration of copper(II) amino acids complexes. *Journal of Computational Chemistry*, 39(14):821–826, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bannerman:2011:DFG

[BSL11] M. N. Bannerman, R. Sargant, and L. Lue. DynamO: a free $O(N)$ general event-driven molecular dynamics simulator. *Journal of Computational Chemistry*, 32(15):3329–3338, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bellinger:2016:IPS

[BSL+16] Daniel Bellinger, Volker Settels, Wenlan Liu, Reinhold F. Fink, and Bernd Engels. Influence of a polarizable surrounding on the electronically excited states of aggregated perylene materials. *Journal of Computational Chemistry*, 37(17):1601–1610, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bomble:2013:BAP

[BSPP+13] Laetitia Bomble, Stephan N. Steinmann, Nancy Perez-Peralta, Gabriel Merino, and Clemence Corminboeuf. Bonding analysis of planar hypercoordinate atoms via the generalized BLW-LOL. *Journal of Computational Chemistry*, 34 (26):2242–2248, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Berenger:2012:SNU

[BSZ+12] Francois Berenger, Rojan Shrestha, Yong Zhou, David Simoncini, and Kam Y. J. Zhang. Software news and updates: Durandal: Fast exact clustering of protein decoys. *Journal of Computational Chemistry*, 33(4):471–474, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bartashevich:2018:CVP

[BT18] Ekaterina Bartashevich and Vladimir Tsirelson. A comparative view on the potential acting on an electron in a molecule and the electrostatic potential through the typical halogen bonds. *Journal of Computational Chemistry*, 39(10):573–580, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bachega:2013:SNU

[BTA+13] José Fernando R. Bachega, Luís Fernando S. M. Timmers, Lucas Assirati, Leonardo R. Bachega, Martin J. Field, and Troy

Wymore. Software news and updates: GTKDynamo: A PyMOL plug-in for QC/MM hybrid potential simulations. *Journal of Computational Chemistry*, 34(25):2190–2196, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bylaska:2011:PIP

[BTB+11] Eric J. Bylaska, Kiril Tsemekhman, Scott B. Baden, John H. Weare, and Hannes Jonsson. Parallel implementation of γ-point pseudopotential plane-wave DFT with exact exchange. *Journal of Computational Chemistry*, 32(1):54–69, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baskaran:2012:FCP

[BTMS12] Sambath Baskaran, Masilamani Tamizmani, Thanigachalam Mahalakshmi, and Chinnappan Sivasankar. A [Fe(CB_6)] platform for binding of small molecules: Insights from DFT calculations. *Journal of Computational Chemistry*, 33(10):1047–1054, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bertran:2010:IDN

[BTT10] Oscar Bertran, S. B. Trickey, and Juan Torras. Incorporation of deMon2k as a new parallel quantum mechanical code for the PUPIL system. *Journal of Computational Chemistry*, 31(14): 2669–2676, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beruski:2014:ACD

[BV14] Otávio Beruski and Luciano N. Vidal. Algorithms for computer detection of symmetry elements in molecular systems. *Journal of Computational Chemistry*, 35(4):290–299, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bultinck:2013:BFI

[BVC13] Patrick Bultinck, Sofie Van Damme, and Andrés Cedillo. Bond Fukui indices: Comparison of frozen molecular orbital and finite differences through Mulliken populations. *Journal of Computational Chemistry*, 34(28):2421–2429, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bellafont:2017:PCL

[BVHI17] Noèlia Pueyo Bellafont, Francesc Viñes, Wolfgang Hieringer, and Francesc Illas. Predicting core level binding energies shifts: Suitability of the projector augmented wave approach as implemented in VASP. *Journal of Computational Chemistry*, 38(8):518–522, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Biswas:2012:SMS

[BVY+12] Pradip K. Biswas, Nadeem A. Vellore, Jeremy A. Yancey, Tugba G. Kucukkal, Galen Collier, Bernard R. Brooks, Steven J. Stuart, and Robert A. Latour. Simulation of multiphase systems utilizing independent force fields to control intraphase and interphase behavior. *Journal of Computational Chemistry*, 33(16):1458–1466, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:2011:EPA

[BW11a] Jon Baker and Krzysztof Wolinski. An efficient parallel algorithm for the calculation of unrestricted canonical MP2 energies. *Journal of Computational Chemistry*, 32(15):3304–3312, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baker:2011:ISU

[BW11b] Jon Baker and Krzysztof Wolinski. Isomerization of stilbene using enforced geometry optimization. *Journal of Computational Chemistry*, 32(1):43–53, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Betz:2015:PAO

[BW15] Robin M. Betz and Ross C. Walker. Paramfit: Automated optimization of force field parameters for molecular dynamics simulations. *Journal of Computational Chemistry*, 36(2):79–87, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bezugly:2010:ELIa

[BWKW10a] Viktor Bezugly, Pawel Wielgus, Miroslav Kohout, and Frank R. Wagner. Electron localizability indicators ELI–D and ELIA for highly correlated wavefunctions of homonuclear dimers. I. Li_2, Be_2, B_2, and C_2. *Journal of Computational*

Chemistry, 31(7):1504–1519, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bezugly:2010:ELIb

[BWKW10b] Viktor Bezugly, Pawel Wielgus, Miroslav Kohout, and Frank R. Wagner. Electron localizability indicators ELI–D and ELIA for highly correlated wavefunctions of homonuclear dimers. II. N_2, O_2, F_2, and Ne_2. *Journal of Computational Chemistry*, 31(12):2273–2285, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brown:2010:MMP

[BWMSM10] Philip Brown, Christopher J. Woods, Simon McIntosh-Smith, and Frederick R. Manby. A massively multicore parallelization of the Kohn–Sham energy gradients. *Journal of Computational Chemistry*, 31(10):2008–2013, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bao:2011:NPE

[BY11] Peng Bao and Zhong-Heng Yu. New procedure to evaluate aromaticity at the density functional theory, Hartree–Fock, and post-self-consistent field levels. *Journal of Computational Chemistry*, 32(2):248–259, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brabec:2016:RCS

[BYE+16] Jiri Brabec, Chao Yang, Evgeny Epifanovsky, Anna I. Krylov, and Esmond Ng. Reduced-cost sparsity-exploiting algorithm for solving coupled-cluster equations. *Journal of Computational Chemistry*, 37(12):1059–1067, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bulik:2013:PDF

[BZB+13] Ireneusz W. Bulik, Robert Zaleśny, Wojciech Bartkowiak, Josep M. Luis, Bernard Kirtman, Gustavo E. Scuseria, Aggelos Avramopoulos, Heribert Reis, and Manthos G. Papadopoulos. Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. *Journal of Computational Chemistry*, 34(20):1775–1784, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brovarets:2014:DTL

[BZH14] Ol'ha O. Brovarets', Roman O. Zhurakivsky, and Dmytro M. Hovorun. Is the DPT tautomerization of the long A·G Watson–Crick DNA base mispair a source of the adenine and guanine mutagenic tautomers? A QM and QTAIM response to the biologically important question. *Journal of Computational Chemistry*, 35(6):451–466, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casanova:2010:SME

[CAA10] David Casanova, Pere Alemany, and Santiago Alvarez. Symmetry measures of the electron density. *Journal of Computational Chemistry*, 31(13):2389–2404, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chong:2016:ISC

[CAD16] Leebyn Chong, Fikret Aydin, and Meenakshi Dutt. Implicit solvent coarse-grained model of polyamidoamine dendrimers: Role of generation and pH. *Journal of Computational Chemistry*, 37(10):920–926, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casanova:2013:PAM

[CAF+13] David Casanova, Pere Alemany, Andrés Falceto, Abel Carreras, and Santiago Alvarez. Pseudosymmetry analysis of molecular orbitals. *Journal of Computational Chemistry*, 34 (15):1321–1331, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cammi:2015:NEP

[Cam15] Roberto Cammi. A new extension of the polarizable continuum model: Toward a quantum chemical description of chemical reactions at extreme high pressure. *Journal of Computational Chemistry*, 36(30):2246–2259, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cammi:2019:RCC

[Cam19] Roberto Cammi. The role of computational chemistry in the experimental determination of the dipole moment of molecules in solution. *Journal of Computational Chemistry*, 40(26):

2309–2317, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Canepa:2010:SWM

[Can10] Carlo Canepa. A stationary-wave model of enzyme catalysis. *Journal of Computational Chemistry*, 31(2):343–350, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [LHMM11] and reply [Can11].

Canepa:2011:RCS

[Can11] Carlo Canepa. Reply to the comment on "A stationary-wave model of enzyme catalysis". *Journal of Computational Chemistry*, 32(2):370–371, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [Can10, LHMM11].

Coe:2017:ICS

[CAP17] Jeremy P. Coe, Nuno M. S. Almeida, and Martin J. Paterson. Investigation of challenging spin systems using Monte Carlo configuration interaction and the density matrix renormalization group. *Journal of Computational Chemistry*, 38 (31):2701–2712, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carlsen:2014:UOE

[Car14] Martin Carlsen. Using operators to expand the block matrices forming the Hessian of a molecular potential. *Journal of Computational Chemistry*, 35(15):1149–1158, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casanova:2013:EIR

[Cas13] David Casanova. Efficient implementation of restricted active space configuration interaction with the hole and particle approximation. *Journal of Computational Chemistry*, 34(9): 720–730, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casanova:2014:HMT

[Cas14] David Casanova. How much tetraradical character is present in the Si_6 Ge_9 cluster? *Journal of Computational Chemistry*, 35(12):944–949, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chilton:2013:SNU

[CAT+13] Nicholas F. Chilton, Russell P. Anderson, Lincoln D. Turner, Alessandro Soncini, and Keith S. Murray. Software news and updates: PHI: a powerful new program for the analysis of anisotropic monomeric and exchange-coupled polynuclear *d*- and *f*-block complexes. *Journal of Computational Chemistry*, 34(13):1164–1175, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Courcot:2011:MIB

[CB11a] Blandine Courcot and Adam J. Bridgeman. Modeling the interactions between polyoxometalates and their environment. *Journal of Computational Chemistry*, 32(15):3143–3153, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Courcot:2011:OMMa

[CB11b] Blandine Courcot and Adam J. Bridgeman. Optimization of a molecular mechanics force field for polyoxometalates based on a genetic algorithm. *Journal of Computational Chemistry*, 32(2):240–247, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Courcot:2011:OMMb

[CB11c] Blandine Courcot and Adam J. Bridgeman. Optimization of a molecular mechanics force field for type-II polyoxometalates focussing on electrostatic interactions: a case study. *Journal of Computational Chemistry*, 32(8):1703–1710, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Czyznikowska:2011:POS

[CB11d] Żaneta Czyżnikowska and Wojciech Bartkowiak. Physical origins of the stability of aromatic amino acid core ring-polycyclic hydrocarbon complexes: a post-Hartree–Fock and density functional study. *Journal of Computational Chemistry*, 32(9):1887–1895, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choudhary:2019:DCM

[CBDS19] VineetKumar Choudhary, ArvindKumar Bhatt, Dibyajit Dash, and Neeraj Sharma. DFT calculations on molecular structures, HOMO–LUMO study, reactivity descriptors and spectral analyses of newly synthesized diorganotin(IV) 2-chloridophenylacetohydroxamate complexes. *Journal of Computational Chemistry*, 40(27):2354–2363, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cumberworth:2016:FES

[CBG16] Alexander Cumberworth, Jennifer M. Bui, and Jörg Gsponer. Free energies of solvation in the context of protein folding: Implications for implicit and explicit solvent models. *Journal of Computational Chemistry*, 37(7):629–640, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakraborty:2017:ESI

[CBG17] Rahul Chakraborty, Samik Bose, and Debashree Ghosh. Effect of solvation on the ionization of guanine nucleotide: a hybrid QM/EFP study. *Journal of Computational Chemistry*, 38(29):2528–2537, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Canneaux:2014:SNU

[CBH14] Sébastien Canneaux, Frédéric Bohr, and Eric Henon. Software news and updates: KiSThelP: a program to predict thermodynamic properties and rate constants from quantum chemistry results. *Journal of Computational Chemistry*, 35(1):82–93, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cailliez:2014:CFM

[CBP14] Fabien Cailliez, Arnaud Bourasseau, and Pascal Pernot. Calibration of forcefields for molecular simulation: Sequential design of computer experiments for building cost-efficient kriging metamodels. *Journal of Computational Chemistry*, 35(2):130–149, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cardone:2015:DCN

[CBP+15] Antonio Cardone, Aaron Bornstein, Harish C. Pant, Mary Brady, Ram Sriram, and Sergio A. Hassan. Detection and characterization of nonspecific, sparsely populated binding modes in the early stages of complexation. *Journal of Computational Chemistry*, 36(13):983–995, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2016:HSC

[CBTZ16] Xi Chen, Fu-Quan Bai, Yongan Tang, and Hong-Xing Zhang. How the substituents in corannulene and sumanene derivatives alter their molecular assemblings and charge transport properties? — A theoretical study with a dimer model. *Journal of Computational Chemistry*, 37(9):813–824, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chuang:2011:IBS

[CC11] Yao-Yuan Chuang and Sheng-Min Chen. Infinite basis set extrapolation for double hybrid density functional theory 1: Effect of applying various extrapolation functions. *Journal of Computational Chemistry*, 32(8):1671–1679, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakraborty:2012:VNL

[CC12a] Debashree Chakraborty and Amalendu Chandra. Voids and necks in liquid ammonia and their roles in diffusion of ions of varying size. *Journal of Computational Chemistry*, 33(8): 843–852, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chys:2012:SPC

[CC12b] Pieter Chys and Pablo Chacón. Spinor product computations for protein conformations. *Journal of Computational Chemistry*, 33(21):1717–1729, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakraborty:2018:CIT

[CC18a] Debdutta Chakraborty and Pratim Kumar Chattaraj. Confinement induced thermodynamic and kinetic facilitation of some Diels–Alder reactions inside a CB[7] cavitand. *Journal of Computational Chemistry*, 39(3):151–160, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakraborty:2018:HGI

[CC18b] Debdutta Chakraborty and Pratim Kumar Chattaraj. Host–guest interactions between octa acid and cations/nucleobases. *Journal of Computational Chemistry*, 39(3):161–175, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakraborty:2018:RIS

[CC18c] Debdutta Chakraborty and Pratim Kumar Chattaraj. Reactions involving some gas molecules through sequestration on Al_{12} Be cluster: an electron density based study. *Journal of Computational Chemistry*, 39(10):535–545, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carnimeo:2015:AGM

[CCB15] Ivan Carnimeo, Chiara Cappelli, and Vincenzo Barone. Analytical gradients for MP2, double hybrid functionals, and TD-DFT with polarizable embedding described by fluctuating charges. *Journal of Computational Chemistry*, 36(31):2271–2290, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2011:MSP

[CCC+11] Duan Chen, Zhan Chen, Changjun Chen, Weihua Geng, and Guo-Wei Wei. MIBPB: a software package for electrostatic analysis. *Journal of Computational Chemistry*, 32(4):756–770, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campo-Cacharron:2014:IAU

[CCCLCGRO14] Alba Campo-Cacharrón, Enrique M. Cabaleiro-Lago, Jorge A. Carrazana-García, and Jesús Rodríguez-Otero. Interaction of aromatic units of amino acids with guanidinium cation: the interplay of $\pi \cdots \pi$, $XH \cdots \pi$ and $M^+ \cdots \pi$ contacts. *Journal of Computational Chemistry*, 35(17):1290–1301, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campo-Cacharron:2014:IBI

[CCCLRO14] Alba Campo-Cacharrón, Enrique M. Cabaleiro-Lago, and Jesús Rodríguez-Otero. Interaction between ions and substituted buckybowls: a comprehensive computational study. *Journal of Computational Chemistry*, 35(21):1533–1544, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:2011:ADN

[CCJ+11] Jee-Gong Chang, Hsin-Tsung Chen, Shin-Pon Ju, Ching-Sheng Chang, and Meng-Hsiung Weng. Adsorption and dissociation of NH_3 on clean and hydroxylated TiO_2 rutile (110) surfaces: a computational study. *Journal of Computational Chemistry*, 32(6):1101–1112, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2010:FPC

[CCJC10] Hsin-Tsung Chen, Jee-Gong Chang, Shin-Pon Ju, and Hui-Lung Chen. First-principle calculations on CO oxidation catalyzed by a gold nanoparticle. *Journal of Computational Chemistry*, 31(2):258–265, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cacelli:2012:AAP

[CCLP12] Ivo Cacelli, Antonella Cimoli, Paolo Roberto Livotto, and Giacomo Prampolini. An automated approach for the parameterization of accurate intermolecular force-fields: Pyridine as a case study. *Journal of Computational Chemistry*, 33(10): 1055–1067, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chattopadhyay:2015:SSM

[CCM15] Sudip Chattopadhyay, Rajat K. Chaudhuri, and Uttam Sinha Mahapatra. State-specific multireference perturbation theory with improved virtual orbitals: Taming the ground state of F_2, Be_2, and N_2. *Journal of Computational Chemistry*, 36 (12):907–925, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chiang:2014:TBH

[CCOH14] Hsin-Lin Chiang, Chun-Jung Chen, Hisashi Okumura, and Chin-Kun Hu. Transformation between α-helix and β-sheet structures of one and two polyglutamine peptides in explicit water molecules by replica-exchange molecular dynamics simulations. *Journal of Computational Chemistry*, 35(19):1430–1437, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cammi:2018:ACP

[CCR18] Roberto Cammi, Bo Chen, and Martin Rahm. Analytical calculation of pressure for confined atomic and molecular systems using the eXtreme-Pressure Polarizable Continuum Model. *Journal of Computational Chemistry*, 39(26):2243–2250, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chiu:2014:PAE

[cCVG+14] Cheng chau Chiu, Georgi N. Vayssilov, Alexander Genest, Armando Borgna, and Notker Rösch. Predicting adsorption enthalpies on silicalite and HZSM-5: a benchmark study on DFT strategies addressing dispersion interactions. *Journal of Computational Chemistry*, 35(10):809–819, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cickovski:2010:MMD

[CCW+10] Trevor Cickovski, Santanu Chatterjee, Jacob Wenger, Christopher R. Sweet, and Jesús A. Izaguirre. MDLab: a molecular dynamics simulation prototyping environment. *Journal of Computational Chemistry*, 31(7):1345–1356, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chiu:2011:DPI

[CCYL11] Shih-Hau Chiu, Chien-Chi Chen, Gwo-Fang Yuan, and Thy-Hou Lin. Deriving the phylogenetic information from some physicochemical properties of protein sequences computed. *Journal of Computational Chemistry*, 32(1):70–80, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2011:EPM

[CD11] Yung-Fou Chen and J. J. Dannenberg. The effect of polarization on multiple hydrogen-bond formation in models of self-assembling materials. *Journal of Computational Chemistry*, 32(13):2890–2895, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2013:NQS

[CD13] Ramon Carbó-Dorca. Notes on quantitative structure–property relationships (QSPR), part 3: Density functions origin shift as a source of quantum QSPR algorithms in molecular spaces. *Journal of Computational Chemistry*, 34(9):766–779, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2016:AQM

[CD16] Ramon Carbó-Dorca. Aromaticity, quantum multimolecular polyhedra, and quantum QSPR fundamental equation. *Journal of Computational Chemistry*, 37(1):78–82, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2019:BRS

[CD19] Ramon Carbó-Dorca. Book review: *"Solved and unsolved problems of structural chemistry"* by Milan Randić, Marjana Novic, and Dejan Plavsić, CRC Press, Boca Raton, 2016, xx + 472 pp. ISBN 13-978-1-4987-1151-7. *Journal of Computational Chemistry*, 40(21):1880, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2010:CQSb

[CDB10] R. Carbó-Dorca and E. Besalú. Communications on quantum similarity (2): a geometric discussion on holographic electron density theorem and confined quantum similarity measures. *Journal of Computational Chemistry*, 31(13):2452–2462, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2011:CQS

[CDBM11] Ramon Carbó-Dorca, Emili Besalú, and Luz Dary Mercado. Communications on quantum similarity, part 3: a geometric-quantum similarity molecular superposition algorithm. *Journal of Computational Chemistry*, 32(4):582–599, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2019:DAP

[CDC19] Ramon Carbó-Dorca and Tanmoy Chakraborty. Divagations about the periodic table: Boolean hypercube and quantum similarity connections. *Journal of Computational Chemistry*, 40(30):2653–2663, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carbo-Dorca:2010:CQSa

[CDM10] Ramon Carbó-Dorca and Luz Dary Mercado. Commentaries on quantum similarity (1): Density gradient quantum similarity. *Journal of Computational Chemistry*, 31(11):2195–2212, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cazals:2015:CES

[CDM+15] Frédéric Cazals, Tom Dreyfus, Dorian Mazauric, Christine-Andrea Roth, and Charles H. Robert. Conformational ensembles and sampled energy landscapes: Analysis and comparison. *Journal of Computational Chemistry*, 36(16):1213–1231, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cheung:2016:PFR

[CDS16] Ngaam J. Cheung, Xue-Ming Ding, and Hong-Bin Shen. Protein folds recognized by an intelligent predictor based-on evolutionary and structural information. *Journal of Computational Chemistry*, 37(4):426–436, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casassa:2015:EDA

[CEBO15] Silvia Casassa, Alessandro Erba, Jacopo Baima, and Roberto Orlando. Electron density analysis of large (molecular and periodic) systems: a parallel implementation. *Journal of Computational Chemistry*, 36(26):1940–1946, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2014:NSE

[CF14] Feiwu Chen and Zhihui Fan. A new size extensive multireference perturbation theory. *Journal of Computational Chemistry*, 35(2):121–129, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2018:MES

[CF18] Wei Chen and Andrew L. Ferguson. Molecular enhanced sampling with autoencoders: On-the-fly collective variable discovery and accelerated free energy landscape exploration. *Journal of Computational Chemistry*, 39(25):2079–2102, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chevrot:2015:ESM

[CFC15] Guillaume Chevrot, Eudes Eterno Fileti, and Vitaly V. Chaban. Enhanced stability of the model mini-protein in amino acid ionic liquids and their aqueous solutions. *Journal of Computational Chemistry*, 36(27):2044–2051, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cesario:2019:RHB

[CFM+19] Diego Cesario, Mariagrazia Fortino, Tiziana Marino, Francesca Nunzi, Nino Russo, and Emilia Sicilia. The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. *Journal of Computational Chemistry*, 40(8):944–951, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Coccia:2012:QMC

[CG12] Emanuele Coccia and Leonardo Guidoni. Quantum Monte Carlo study of the retinal minimal model $C_5H_6NH_2^+$. *Journal of Computational Chemistry*, 33(29):2332–2339, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carlin:2015:ICA

[CG15] Caleb Carlin and Mark S. Gordon. Ab initio calculation of anion proton affinity and ionization potential for energetic ionic liquids. *Journal of Computational Chemistry*, 36(9):597–600, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakravorty:2019:GBA

[CGA19] Arghya Chakravorty, Emilio Gallicchio, and Emil Alexov. A grid-based algorithm in conjunction with a Gaussian-based model of atoms for describing molecular geometry. *Journal* of Computational Chemistry, 40(12):1290–1304, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choi:2013:SBR

[CGBK13] Yoonjoo Choi, Karl E. Griswold, and Chris Bailey-Kellogg. Structure-based redesign of proteins for minimal T-cell epitope content. *Journal of Computational Chemistry*, 34(10): 879–891, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cantatore:2012:SMP

[CGP12] Valentina Cantatore, Giovanni Granucci, and Maurizio Persico. Stochastic model for photoinduced anisotropy. *Journal of Computational Chemistry*, 33(10):1015–1022, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chaudret:2011:MBE

[CGPP11] Robin Chaudret, Nohad Gresh, Olivier Parisel, and Jean-Philip Piquemal. Many-body exchange-repulsion in polarizable molecular mechanics. I. orbital-based approximations and applications to hydrated metal cation complexes. *Journal of Computational Chemistry*, 32(14):2949–2957, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2016:IPM

[CGR16] Bun Chan, Lars Goerigk, and Leo Radom. On the inclusion of post-MP2 contributions to double-hybrid density functionals. *Journal of Computational Chemistry*, 37(2):183–193, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carreon-Gonzalez:2019:TPS

[CGVBAI19] Mirzam Carreon-Gonzalez, Annik Vivier-Bunge, and Juan Raul Alvarez-Idaboy. Thiophenols, promising scavengers of peroxyl radicals: Mechanisms and kinetics. *Journal of Computational Chemistry*, 40(24):2103–2110, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chidthong:2010:ESP

[CH10] Rungtiwa Chidthong and Supa Hannongbua. Excited state properties, fluorescence energies, and lifetimes of a poly(fluorene-phenylene), based on TD-DFT investigation. *Journal of Computational Chemistry*, 31(7):1450–1457, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chong:2014:SDA

[CH14] Song-Ho Chong and Sihyun Ham. Site-directed analysis on protein hydrophobicity. *Journal of Computational Chemistry*, 35(18):1364–1370, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2016:WFE

[CH16] Changjun Chen and Yanzhao Huang. Walking freely in the energy and temperature space by the modified replica exchange molecular dynamics method. *Journal of Computational Chemistry*, 37(17):1565–1575, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:2013:AAC

[CHC+13] Jia-Lin Chang, Cyong-Huei Huang, Sue-Chang Chen, Tsung-Hao Yin, and Yi-Tsung Chen. An analytical approach for computing Franck–Condon integrals of harmonic oscillators with arbitrary dimensions. *Journal of Computational Chemistry*, 34(9):757–765, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2017:CMF

[Che17] Changjun Chen. Constructing a multidimensional free energy surface like a spider weaving a web. *Journal of Computational Chemistry*, 38(27):2298–2306, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2016:HEI

[CHG+16] Yixiang Cao, Thomas Hughes, Dave Giesen, Mathew D. Halls, Alexander Goldberg, Tati Reddy Vadicherla, Madhavi Sastry, Bhargav Patel, Woody Sherman, Andrew L. Weisman, and Richard A. Friesner. Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. *Journal of Computational Chemistry*, 37(16):1425–1441, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cilpa:2010:AIC

[CHKR10] G. Cilpa, M. T. Hyvönen, A. Koivuniemi, and M.-L. Riekkola. Atomistic insight into chondroitin-6-sulfate glycosaminoglycan chain through quantum mechanics calculations and molecular dynamics simulation. *Journal of Computational Chemistry*, 31(8):1670–1680, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Czajlik:2011:LPB

[CHP11] András Czajlik, Ilona Hudáky, and András Perczel. Local protein backbone folds determined by calculated NMR chemical shifts. *Journal of Computational Chemistry*, 32(16):3362–3382, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chiba:2012:EPL

[CHR+12a] Shuntaro Chiba, Yuich Harano, Roland Roth, Masahiro Kinoshita, and Minoru Sakurai. Evaluation of protein-ligand binding free energy focused on its entropic components. *Journal of Computational Chemistry*, 33(5):550–560, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [CHR+12b].

Chiba:2012:EEP

[CHR+12b] Shuntaro Chiba, Yuichi Harano, Roland Roth, Masahiro Kinoshita, and Minoru Sakurai. Errata: "Evaluation of protein-ligand binding free energy focused on its entropic components" [J. Comp. Chem. **33**, 550–560]. *Journal of Computational Chemistry*, 33(27):2210, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [CHR+12a].

Chu:2010:QMQ

[Chu10] Tianshu Chu. Quantum mechanics and quasiclassical study of the H/D + FO $\rightarrow$ OH/OD + F, HF/DF + O reactions: Chemical stereodynamics. *Journal of Computational Chemistry*, 31(7):1385–1396, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chang:2013:PSF

[CIKT13] Le Chang, Takeshi Ishikawa, Kazuo Kuwata, and Shoji Takada. Protein-specific force field derived from the fragment molecular orbital method can improve protein–ligand binding interactions. *Journal of Computational Chemistry*, 34(14):1251–1257, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2013:PPD

[CJL+13] Zhanghui Chen, Xiangwei Jiang, Jingbo Li, Shushen Li, and Linwang Wang. PDECO: Parallel differential evolution for clusters optimization. *Journal of Computational Chemistry*, 34(12):1046–1059, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clemente-Juan:2018:VPT

[CJPTC18] Juan M. Clemente-Juan, Andrew Palii, Boris Tsukerblat, and Eugenio Coronado. VIBPACK: a package to treat multidimensional electron-vibrational molecular problems with application to magnetic and optical properties. *Journal of Computational Chemistry*, 39(22):1815–1827, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Condic-Jurkic:2010:CQM

[CJZS10] Karmen Condic-Jurkic, Hendrik Zipse, and David M. Smith. A compound QM/MM procedure: Comparative performance on a pyruvate formate-lyase model system. *Journal of Computational Chemistry*, 31(5):1024–1035, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campen:2010:IES

[CK10] Richard Kramer Campen and James D. Kubicki. Interaction energy and the shift in OH stretch frequency on hydrogen bonding for the $H_2O \to H_2O$, $CH_3OH \to H_2O$, and $H_2O \to CH_3OH$ dimers. *Journal of Computational Chemistry*, 31(5): 963–972, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cvitkovic:2017:DME

[CK17] John P. Cvitkovic and George A. Kaminski. Developing multisite empirical force field models for Pt(II) and cisplatin. *Jour-*

nal of Computational Chemistry*, 38(3):161–168, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cummins:2018:RMC

[CKG18] Peter L. Cummins, Babu Kannappan, and Jill E. Gready. Revised mechanism of carboxylation of ribulose-1,5-biphosphate by Rubisco from large scale quantum chemical calculations. *Journal of Computational Chemistry*, 39(21):1656–1665, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2017:CFS

[CKH17] Bun Chan, Yukio Kawashima, and Kimihiko Hirao. Correlation functional in screened-exchange density functional theory procedures. *Journal of Computational Chemistry*, 38(27): 2307–2315, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2019:RTR

[CKH19] Bun Chan, Yukio Kawashima, and Kimihiko Hirao. The reHISS Three-Range Exchange Functional with an Optimal Variation of Hartree–Fock and Its Use in the reHISSB-D Density Functional Theory Method. *Journal of Computational Chemistry*, 40(1):29–38, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choi:2016:PHC

[CKKK16] Sunghwan Choi, Oh-Kyoung Kwon, Jaewook Kim, and Woo Youn Kim. Performance of heterogeneous computing with graphics processing unit and many integrated core for Hartree potential calculations on a numerical grid. *Journal of Computational Chemistry*, 37(24):2193–2201, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2011:RBS

[CKL$^+$11] Jun-Xian Chen, Chang Kon Kim, Hai Whang Lee, Ying Xue, and Chan Kyung Kim. Reexamination of the π-bond strengths within $H_2C{=\!=}XH_n$ systems: a theoretical study. *Journal of Computational Chemistry*, 32(7):1361–1367, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choi:2010:NAD

[CKP10] Hwanho Choi, Hongsuk Kang, and Hwangseo Park. New angle-dependent potential energy function for backbone–backbone hydrogen bond in protein–protein interactions. *Journal of Computational Chemistry*, 31(5):897–903, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2016:NMA

[CL16] Zhenlian Chen and Jun Li. A new method applicable to study solid compounds with multiple polyhedral structures. *Journal of Computational Chemistry*, 37(16):1476–1483, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chakavorty:2016:ECB

[CLA16] Arghya Chakavorty, Lin Li, and Emil Alexov. Electrostatic component of binding energy: Interpreting predictions from Poisson–Boltzmann equation and modeling protocols. *Journal of Computational Chemistry*, 37(28):2495–2507, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chung:2011:CST

[CLC11] Yi-Hsing Chung, Arvin Huang-Te Li, and Sheng D. Chao. Computer simulation of trifluoromethane properties with ab initio force field. *Journal of Computational Chemistry*, 32(11): 2414–2421, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cabaleiro-Lago:2018:DCC

[CLFRO18] Enrique M. Cabaleiro-Lago, Berta Fernández, and Jesús Rodríguez-Otero. Dissecting the concave–convex π–π interaction in corannulene and sumanene dimers: SAPT(DFT) analysis and performance of DFT dispersion-corrected methods. *Journal of Computational Chemistry*, 39(2):93–104, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Click:2011:QRN

[CLK11] Timothy H. Click, Aibing Liu, and George A. Kaminski. Quality of random number generators significantly affects results of

Monte Carlo simulations for organic and biological systems. *Journal of Computational Chemistry*, 32(3):513–524, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Clote:2015:EDR

[Clo15] Peter Clote. Expected degree for RNA secondary structure networks. *Journal of Computational Chemistry*, 36(2):103–117, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2010:NSO

[CLX+10] Dong-Sheng Cao, Yi-Zeng Liang, Qing-Song Xu, Hong-Dong Li, and Xian Chen. A new strategy of outlier detection for QSAR/QSPR. *Journal of Computational Chemistry*, 31(3): 592–602, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campana:2013:TMP

[CM13a] Carlos Campañá and Ronald E. Miller. Transiting the molecular potential energy surface along low energy pathways: The TRREAT algorithm. *Journal of Computational Chemistry*, 34 (29):2502–2513, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chitsaz:2013:GHR

[CM13b] Mohsen Chitsaz and Stephen L. Mayo. GRID: a high-resolution protein structure refinement algorithm. *Journal of Computational Chemistry*, 34(6):445–450, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cukrowski:2016:IQF

[CM16] Ignacy Cukrowski and Paidamwoyo Mangondo. Interacting quantum fragments-rooted preorganized-interacting fragments attributed relative molecular stability of the Be^{II} complexes of nitrilotriacetic acid and nitrilotri-3-propionic acid. *Journal of Computational Chemistry*, 37(15):1373–1387, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cendic:2013:MMC

[ĆMD13] Marina Ćendić, Zoran D. Matović, and Robert J. Deeth. Molecular modeling for Cu(II)-aminopolycarboxylate complexes: Structures, conformational energies, and ligand binding affinities. *Journal of Computational Chemistry*, 34(31): 2687–2696, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Calzado:2011:HBS

[CME11] Carmen J. Calzado, A. Monari, and S. Evangelisti. Heisenberg behavior of some carbon-beryllium compounds: How well truncated-CI approaches work. *Journal of Computational Chemistry*, 32(2):315–324, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campetella:2017:CTE

[CMF+17] Marco Campetella, Federica Maschietto, Mike J. Frisch, Giovanni Scalmani, Ilaria Ciofini, and Carlo Adamo. Charge transfer excitations in TDDFT: a ghost-hunter index. *Journal of Computational Chemistry*, 38(25):2151–2156, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Calborean:2018:CMP

[CMM18] Adrian Calborean, Cristian Morari, and Pascale Maldivi. Combined molecular and periodic DFT analysis of the adsorption of Co macrocycles on graphene. *Journal of Computational Chemistry*, 39(2):130–138, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Comba:2013:EFC

[CMS13] Peter Comba, Bodo Martin, and Avik Sanyal. An efficient fluctuating charge model for transition metal complexes. *Journal of Computational Chemistry*, 34(18):1598–1608, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Christ:2010:BIF

[CMvG10] Clara D. Christ, Alan E. Mark, and Wilfred F. van Gunsteren. Basic ingredients of free energy calculations: a review. *Journal of Computational Chemistry*, 31(8):1569–1582, June

2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Csonka:1997:STD

[CNK97] Gábor I. Csonka, Nam Anh Nguyen, and István Kolossváry. Simple tests for density functional methods. *Journal of Computational Chemistry*, 18(12):1534–1545, September 1997. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cohen:2018:EPP

[Coh18] Leon Cohen. The eigenvalue problem in phase space. *Journal of Computational Chemistry*, 39(17):1059–1067, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chiba:2019:FFP

[COHI19] Shuntaro Chiba, Yasushi Okuno, Teruki Honma, and Mitsunori Ikeguchi. Force-field parametrization based on radial and energy distribution functions. *Journal of Computational Chemistry*, 40(29):2577–2585, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cooper:2019:BIA

[Coo19] Christopher D. Cooper. A boundary-integral approach for the Poisson–Boltzmann equation with polarizable force fields. *Journal of Computational Chemistry*, 40(18):1680–1692, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Corni:2017:LER

[Cor17] Stefano Corni. Letters to the Editor: Reply to “Molecular mechanics models for the image charge”. *Journal of Computational Chemistry*, 38(24):2130–2133, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SFLG+17].

Cardamone:2015:PCD

[CP15] Salvatore Cardamone and Paul L. A. Popelier. Prediction of conformationally dependent atomic multipole moments in carbohydrates. *Journal of Computational Chemistry*, 36(32): 2361–2373, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Click:2012:IEP

[CPK12] Timothy H. Click, Sergei Y. Ponomarev, and George A. Kaminski. Importance of electrostatic polarizability in calculating cysteine acidity constants and copper(I) binding energy of *Bacillus subtilis* CopZ. *Journal of Computational Chemistry*, 33(11):1142–1151, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cvitkovic:2019:PCG

[CPK19] John P. Cvitkovic, Connor D. Pauplis, and George A. Kaminski. PKA17 — a coarse-grain grid-based methodology and web-based software for predicting protein pK_a shifts. *Journal of Computational Chemistry*, 40(18):1718–1726, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cui:2011:EMT

[CPLL11] Feng-Chao Cui, Xiao-Liang Pan, Wei Liu, and Jing-Yao Liu. Elucidation of the methyl transfer mechanism catalyzed by chalcone O-methyltransferase: a density functional study. *Journal of Computational Chemistry*, 32(14):3068–3074, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Charistos:2017:COC

[CPN+17] Nickolas D. Charistos, Anastasios G. Papadopoulos, Thomas A. Nikopoulos, Alvaro Muñoz-Castro, and Michael P. Sigalas. Canonical orbital contributions to the magnetic fields induced by global and local diatropic and paratropic ring currents. *Journal of Computational Chemistry*, 38(30):2594–2604, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Caruso:2018:XRC

[CPR18] Francesco Caruso, Sarah Paumier, and Miriam Rossi. X-ray Crystal Structure of Embelin and Its DFT Scavenging of Superoxide Radical. *Journal of Computational Chemistry*, 39 (18):1143–1148, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Calvello:2018:CIC

[CPRS18] Simone Calvello, Matteo Piccardo, Shashank Vittal Rao, and Alessandro Soncini. CERES: an ab initio code dedicated to the calculation of the electronic structure and magnetic properties of lanthanide complexes. *Journal of Computational Chemistry*, 39(6):328–337, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chaiwongwattana:2012:DMS

[CPV+12] Sermsiri Chaiwongwattana, Mayuree Phonyiem, Viwat Vchirawongkwin, Supakit Prueksaaroon, and Kritsana Sagarik. Dynamics and mechanism of structural diffusion in linear hydrogen bond. *Journal of Computational Chemistry*, 33(2): 175–188, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campeggio:2019:DCD

[CPZ19] Jonathan Campeggio, Antonino Polimeno, and Mirco Zerbetto. DiTe2: Calculating the diffusion tensor for flexible molecules. *Journal of Computational Chemistry*, 40(4):697–705, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2010:PIB

[CQFC10] Lei Chen, Ziliang Qian, Kaiyan Fen, and Yudong Cai. Prediction of interactiveness between small molecules and enzymes by combining gene ontology and compound similarity. *Journal of Computational Chemistry*, 31(8):1766–1776, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carter:2014:VWC

[CR14] Damien J. Carter and Andrew L. Rohl. van der Waals corrected density functional calculations of the adsorption of benzene on the Cu (111) surface. *Journal of Computational Chemistry*, 35(31):2263–2271, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2019:OIE

[CR19] Bun Chan and Leo Radom. An ONIOM investigation of the effect of conformation on bond dissociation energies in peptides. *Journal of Computational Chemistry*, 40(1):82–88, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Castro:2013:SMD

[CRC13] Maria Ana Castro, Adrian E. Roitberg, and Fabio D. Cukiernik. Simulation of mesogenic diruthenium tetracarboxylates: Development of a force field for coordination polymers of the MMX type. *Journal of Computational Chemistry*, 34(15):1283–1290, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cormanich:2016:IIC

[CROB16] Rodrigo A. Cormanich, Roberto Rittner, David O'Hagan, and Michael Bühl. Inter- and intramolecular CF$\cdots$C$=$O interactions on aliphatic and cyclohexane carbonyl derivatives. *Journal of Computational Chemistry*, 37(1):25–33, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2018:MAA

[CRZ+18] Xiaofang Cao, Chunying Rong, Aiguo Zhong, Tian Lu, and Shubin Liu. Molecular acidity: an accurate description with information-theoretic approach in density functional reactivity theory. *Journal of Computational Chemistry*, 39(2):117–129, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2014:ESN

[CS14] Wei Chen and Jana K. Shen. Effects of system net charge and electrostatic truncation on all-atom constant pH molecular dynamics. *Journal of Computational Chemistry*, 35(27):1986–1996, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cheron:2017:ESB

[CS17] Nicolas Chéron and Eugene I. Shakhnovich. Effect of sampling on BACE-1 ligands binding free energy predictions via MM–PBSA calculations. *Journal of Computational Chemistry*, 38 (22):1941–1951, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carvalho-Silva:2017:DTS

[CSAdOM17] Valter H. Carvalho-Silva, Vincenzo Aquilanti, Heibbe C. B. de Oliveira, and Kleber C. Mundim. Deformed transition-state theory: Deviation from Arrhenius behavior and application to bimolecular hydrogen transfer reaction rates in the tunneling regime. *Journal of Computational Chemistry*, 38 (3):178–188, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2018:RDH

[CSC+18] Xian Chen, Jian Song, Zhe-Ning Chen, Tan Jin, Fengqin Long, Hua Xie, Yisong Zheng, Wei Zhuang, and Lu Zhang. Rational designing of 8-hydroxyquinolin-imidazolinone-based fluorescent protein mutants with dramatically red shifted emission: a computational study. *Journal of Computational Chemistry*, 39(27):2307–2315, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cardona-Serra:2016:SNU

[CSEMB+16] Salvador Cardona-Serra, Luis Escalera-Moreno, José J. Baldoví, Alejandro Gaita-Ariño, Juan M. Clemente-Juan, and Eugenio Coronado. Software news and updates: SIMPRE1.2: Considering the hyperfine and quadrupolar couplings and the nuclear spin bath decoherence. *Journal of Computational Chemistry*, 37(13):1238–1244, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Calbo:2017:DCS

[CSGOA17] Joaquín Calbo, Juan C. Sancho-García, Enrique Ortí, and Juan Aragó. DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes. *Journal of Computational Chemistry*, 38(21):1869–1878, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2015:TCR

[CSKH15] Bun Chan, Jong-Won Song, Yukio Kawashima, and Kimihiko Hirao. Toward the complete range separation of non-hybrid exchange–correlation functional. *Journal of Computational Chemistry*, 36(12):871–877, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2016:POC

[CSKH16] Bun Chan, Jong-Won Song, Yukio Kawashima, and Kimihiko Hirao. Performance of the OP correlation functional in relation to its formulation: Influence of the exchange component and the effect of incorporating same-spin correlations. *Journal of Computational Chemistry*, 37(14):1306–1312, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cukrowski:2016:SCT

[CSM16] Ignacy Cukrowski, Filip Sagan, and Mariusz Paweł Mitoraj. On the stability of cis- and trans-2-butene isomers. An insight based on the FAMSEC, IQA, and ETS-NOCV schemes. *Journal of Computational Chemistry*, 37(32):2783–2798, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Coutinho:2018:KOH

[CSNCS+18] Nayara D. Coutinho, Flavio O. Sanches-Neto, Valter H. Carvalho-Silva, Heibbe C. B. de Oliveira, Luiz A. Ribeiro, and Vincenzo Aquilanti. Kinetics of the OH + HCl $\rightarrow$ H_2O + Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. *Journal of Computational Chemistry*, 39(30):2508–2516, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cardona-Serra:2017:IDI

[CSS17] Salvador Cardona-Serra and Stefano Sanvito. Influence of the dipolar interactions on the relative stability in spin crossover systems. *Journal of Computational Chemistry*, 38(4):224–227, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Collignon:2011:TPM

[CSSB11] Barbara Collignon, Roland Schulz, Jeremy C. Smith, and Jerome Baudry. Task-parallel message passing interface implementation of Autodock4 for docking of very large databases of compounds using high-performance super-computers. *Journal of Computational Chemistry*, 32(6):1202–1209, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2017:APE

[CSXZ17] Jun Chen, Neil Qiang Su, Xin Xu, and Dong H. Zhang. Accurate potential energy surfaces for hydrogen abstraction reactions: a benchmark study on the XYG3 doubly hybrid density functional. *Journal of Computational Chemistry*, 38(27): 2326–2334, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Coe:2013:MCC

[CTP13] Jeremy P. Coe, Daniel J. Taylor, and Martin J. Paterson. Monte Carlo configuration interaction applied to multipole moments, ionisation energies and electron affinities. *Journal of Computational Chemistry*, 34(13):1083–1093, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carvalho:2013:PMD

[CTR13] Alexandra T. P. Carvalho, Ana F. S. Teixeira, and Maria J. Ramos. Parameters for molecular dynamics simulations of iron-sulfur proteins. *Journal of Computational Chemistry*, 34 (18):1540–1548, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Costanzi:2012:SSA

[CV12] Stefano Costanzi and Santiago Vilar. In Silico screening for agonists and blockers of the β_2 adrenergic receptor: Implications of inactive and activated state structures. *Journal of Computational Chemistry*, 33(5):561–572, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chuev:2014:ESS

[CVG14] Gennady N. Chuev, Ivan Vyalov, and Nikolaj Georgi. Extraction of site–site bridge functions and effective pair potentials from simulations of polar molecular liquids. *Journal of Computational Chemistry*, 35(13):1010–1023, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cates:2019:HBH

[CvM19] Emma L. Cates and Tanja van Mourik. Halogen bonding with the halogenabenzene bird structure, halobenzene, and halocyclopentadiene. *Journal of Computational Chemistry*, 40(24):2111–2118, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chavent:2011:GAA

[CVT+11] Matthieu Chavent, Antoine Vanel, Alex Tek, Bruno Levy, Sophie Robert, Bruno Raffin, and Marc Baaden. GPU-accelerated atom and dynamic bond visualization using hyperballs: a unified algorithm for balls, sticks, and hyperboloids. *Journal of Computational Chemistry*, 32(13):2924–2935, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Coutsias:2019:RS

[CW19] Evangelos A. Coutsias and Michael J. Wester. RMSD and symmetry. *Journal of Computational Chemistry*, 40(15):1496–1508, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chai:2011:DFT

[CWHH11] Shuo Chai, Shu-Hao Wen, Jin-Dou Huang, and Ke-Li Han. Density functional theory study on electron and hole transport properties of organic pentacene derivatives with electron-withdrawing substituent. *Journal of Computational Chemistry*, 32(15):3218–3225, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2012:TIP

[CWT+12] Qi Cao, Jing Wang, Zhao-Shuo Tian, Zai-Feng Xie, and Fu-Quan Bai. Theoretical investigation on the photophysical properties of N-heterocyclic carbene iridium (III) complexes $(\mathrm{fpmb})_x$ $\mathrm{Ir(bptz)}_{3-x}$ (x = 1–2). *Journal of Computational Chemistry*, 33(10):1038–1046, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cui:2010:SRE

[CWZB10] Peng Cui, Jian Wu, Guiqing Zhang, and Russell J. Boyd. A simple representation of energy matrix elements in terms of symmetry-invariant bases. *Journal of Computational Chemistry*, 31(3):492–496, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2010:AFE

[CX10] Changjun Chen and Yi Xiao. Accurate free energy calculation along optimized paths. *Journal of Computational Chemistry*, 31(7):1368–1375, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cui:2019:BSP

[CXD+19] Cheng-Xing Cui, Dongdong Xu, Bo-Wen Ding, Ling-Bo Qu, Yu-Ping Zhang, and Yu Lan. Benchmark study of popular density functionals for calculating binding energies of three-center two-electron bonds. *Journal of Computational Chemistry*, 40(4):657–670, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Christodouleas:2010:TBE

[CXS10] Christos Christodouleas, Demetrios Xenides, and Theodore E. Simos. Trends of the bonding effect on the performance of DFT methods in electric properties calculations: a pattern recognition and metric space approach on some XY_2 (X = O, S and Y = H, O, F, S, Cl) molecules. *Journal of Computational Chemistry*, 31(2):412–420, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2014:MRQ

[CXW14] Jie Chen, Yulong Xu, and Dunyou Wang. A multilayered representation, quantum mechanical and molecular mechanics study of the $CH_3F + OH^-$ reaction in water. *Journal of Computational Chemistry*, 35(6):445–450, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2009:PRW

[CY09] Mengen Chen and Wei Yang. On-the-path random walk sampling for efficient optimization of minimum free-energy path. *Journal of Computational Chemistry*, 30(11):1649–1653, August 2009. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [CY13].

Chen:2013:EPR

[CY13] M. E. Chen and W. Yang. Erratum: On-the-path random walk sampling for efficient optimization of minimum free energy path. *Journal of Computational Chemistry*, 34(27):

2400, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [CY09].

Chen:2015:FFD

[CYG+15] Siyan Chen, Shasha Yi, Wenmei Gao, Chuncheng Zuo, and Zhonghan Hu. Force field development for organic molecules: Modifying dihedral and $1-n$ pair interaction parameters. *Journal of Computational Chemistry*, 36(6):376–384, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chintapalli:2010:CLF

[CYI+10] Sree V. Chintapalli, Boon K. Yew, Christopher J. R. Illingworth, Graham J. G. Upton, Philip J. Reeves, Kevin E. B. Parkes, Christopher R. Snell, and Christopher A. Reynolds. Closed loop folding units from structural alignments: Experimental foldons revisited. *Journal of Computational Chemistry*, 31(15):2689–2701, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2017:MII

[CYY+17] Shanshan Cao, Haiyan Yuan, Yang Yang, Mang Wang, Xiaoying Zhang, and Jingping Zhang. Mechanistic investigation inspired "on water" reaction for hydrobromic acid-catalyzed Friedel–Crafts-type reaction of β-naphthol and formaldehyde. *Journal of Computational Chemistry*, 38(26):2268–2275, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cheron:2017:SNU

[CZAF17] Jean-Baptiste Chéron, Martin Zacharias, Serge Antonczak, and Sébastien Fiorucci. Software news and updates: Update of the ATTRACT force field for the prediction of protein–protein binding affinity. *Journal of Computational Chemistry*, 38(21):1887–1890, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chandra:2012:TII

[CZH12] Asit K. Chandra and Thérèse Zeegers-Huyskens. A theoretical investigation of the interaction between substituted carbonyl derivatives and water: Open or cyclic complexes? *Journal of Computational Chemistry*, 33(11):1131–1141, April 30, 2012.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Curco:2011:SSA

[CZNA11] David Curcó, David Zanuy, Ruth Nussinov, and Carlos Alemán. A simulation strategy for the atomistic modeling of flexible molecules covalently tethered to rigid surfaces: Application to peptides. *Journal of Computational Chemistry*, 32(4):607–619, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2011:EMB

[CZY11] Shu-Ling Chen, Dong-Xia Zhao, and Zhong-Zhi Yang. An estimation method of binding free energy in terms of ABEEM$\sigma\pi$ /MM and continuum electrostatics fused into LIE method. *Journal of Computational Chemistry*, 32(2):338–348, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2019:TEG

[CZZL19] Xin Chen, Ya-Fan Zhao, Yang-Yang Zhang, and Jun Li. TGMin: an efficient global minimum searching program for free and surface-supported clusters. *Journal of Computational Chemistry*, 40(10):1105–1112, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dickson:2016:CFB

[DAB16] Alex Dickson, Logan S. Ahlstrom, and Charles L. Brooks III. Coupled folding and binding with 2D Window-Exchange Umbrella Sampling. *Journal of Computational Chemistry*, 37(6): 587–594, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deAngulo:2012:RCA

[dACP12] V. Ruiz de Angulo, J. Cortés, and J. M. Porta. Rigid-CLL: Avoiding constant-distance computations in cell linked-lists algorithms. *Journal of Computational Chemistry*, 33(3):294–300, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Domingo:2015:ERT

[DAdGR15] Alex Domingo, Celestino Angeli, Coen de Graaf, and Vincent Robert. Electronic reorganization triggered by electron transfer: the intervalence charge transfer of a Fe^{3+} /Fe^{2+} bimetallic complex. *Journal of Computational Chemistry*, 36(11): 861–869, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeSilva:2019:ASE

[DAG19] Nuwan De Silva, Matthew A. Adreance, and Mark S. Gordon. Application of a semi-empirical dispersion correction for modeling water clusters. *Journal of Computational Chemistry*, 40(2):310–315, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deAndrade:2015:EMR

[dALdS+15] Railton Barbosa de Andrade, Ezequiel Fragoso Vieira Leitão, Miguel Angelo Fonseca de Souza, Elizete Ventura, and Silmar Andrade do Monte. Effect of methylation on relative energies of tautomers and on the intramolecular proton transfer barriers of protonated nitrosamine: a MR–CISD study. *Journal of Computational Chemistry*, 36(27):2027–2036, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dandu:2018:PDF

[DAP+18] Naveen K. Dandu, Olajumoke Adeyiga, Dipak Panthi, Shaina A. Bird, and Samuel O. Odoh. Performance of density functional theory for describing hetero-metallic active-site motifs for methane-to-methanol conversion in metal-exchanged zeolites. *Journal of Computational Chemistry*, 39 (32):2667–2678, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DAlessando:2015:EDS

[DASA15] Maira D'Alessando, Andrea Amadei, Mauro Stener, and Massimiliano Aschi. Essential dynamics for the study of microstructures in liquids. *Journal of Computational Chemistry*, 36(6):399–407, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dracinsky:2012:VAC

[DB12] Martin Dračínský and Petr Bouř. Vibrational averaging of the chemical shift in crystalline α-glycine. *Journal of Computational Chemistry*, 33(10):1080–1089, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DiPasquale:2016:SNU

[DBDP16] Nicodemo Di Pasquale, Michael Bane, Stuart J. Davie, and Paul L. A. Popelier. Software news and updates: FEREBUS: Highly parallelized engine for kriging training. *Journal of Computational Chemistry*, 37(29):2606–2616, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dutra:2014:LLL

[DBF14] José Diogo L. Dutra, Thiago D. Bispo, and Ricardo O. Freire. LUMPAC lanthanide luminescence software: Efficient and user friendly. *Journal of Computational Chemistry*, 35(10): 772–775, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deshmukh:2011:IHB

[DBG11] Milind M. Deshmukh, Libero J. Bartolotti, and Shridhar R. Gadre. Intramolecular hydrogen bond energy and cooperative interactions in α-, β-, and γ-cyclodextrin conformers. *Journal of Computational Chemistry*, 32(14):2996–3004, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Diaz:2017:END

[DBGO+17] Silvia Díaz, Mateusz Z. Brela, Soledad Gutiérrez-Oliva, Alejandro Toro-Labbé, and Artur Michalak. ETS-NOCV decomposition of the reaction force: The HCN/CNH isomerization reaction assisted by water. *Journal of Computational Chemistry*, 38(24):2076–2087, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dickson:2017:OAS

[DBK17] Alex Dickson, Christopher T. Bailey, and John Karanicolas. Optimal allosteric stabilization sites using contact stabilization analysis. *Journal of Computational Chemistry*, 38(15): 1138–1146, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Demichelis:2015:FPM

[DBM+15] Raffaella Demichelis, Marco Bruno, Francesco R. Massaro, Mauro Prencipe, Marco De La Pierre, and Fabrizio Nestola.

First-principle modelling of forsterite surface properties: Accuracy of methods and basis sets. *Journal of Computational Chemistry*, 36(19):1439–1445, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DiTommaso:2017:TAP

[DBM+17] Stefania Di Tommaso, Diane Bousquet, Delphine Moulin, Frédéric Baltenneck, Priscilla Riva, Hervé David, Aziz Fadli, Jérôme Gomar, Ilaria Ciofini, and Carlo Adamo. Theoretical approaches for predicting the color of rigid dyes in solution. *Journal of Computational Chemistry*, 38(13):998–1004, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Drujon:2013:PHC

[DC13] J. Drujon and Y. Carissan. Pseudopotentials for hybridized carbon atoms. *Journal of Computational Chemistry*, 34(1): 49–59, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deCourcy:2015:BOQ

[dCDP15] Benoit de Courcy, Etienne Derat, and Jean-Philip Piquemal. Bridging organometallics and quantum chemical topology: Understanding electronic relocalisation during palladium-catalyzed reductive elimination. *Journal of Computational Chemistry*, 36(15):1167–1175, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gouveia:2019:DAL

[dCGCRN19] Tiago Leyser da Costa Gouveia, Renan Borsoi Campos, Ronny Rocha Ribeiro, and Fábio Souza Nunes. DFT analysis of the linkage isomerism in penta(ammine)ruthenium(II/III) complexes of benzotriazole: Natural bond orbital method approach and a comprehensive energy decomposition analysis. *Journal of Computational Chemistry*, 40(16):1593–1598, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dong:2012:BCE

[DCHL12] Hua Dong, Bo-Zhen Chen, Ming-Bao Huang, and Roland Lindh. The Bergman cyclizations of the enediyne and its N-substituted analogs using multiconfigurational second-order perturbation theory. *Journal of Computational Chemistry*, 33(5):537–549, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deCarvalho:2013:ICP

[dCLFGL13] Ranieri V. de Carvalho, Daniel Lopez-Ferrer, Katia S. Guimarães, and Roberto D. Lins. IMSPeptider: a computational peptide collision cross-section area calculator based on a novel molecular dynamics simulation protocol. *Journal of Computational Chemistry*, 34(20):1707–1718, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLaPierre:2013:UIM

[DCOD13] Marco De La Pierre, Cédric Carteret, Roberto Orlando, and Roberto Dovesi. Use of ab initio methods for the interpretation of the experimental IR reflectance spectra of crystalline compounds. *Journal of Computational Chemistry*, 34(17): 1476–1485, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deCarvalho:2018:EMT

[dCRN18] E. F. V. de Carvalho and O. Roberto-Neto. Effects of multidimensional tunneling in the kinetics of hydrogen abstraction reactions of $O(^3P)$ with CH_3OCHO. *Journal of Computational Chemistry*, 39(20):1424–1432, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dubaj:2015:IIM

[DCŠ15] Tibor Dubaj, Zuzana Cibulková, and Peter Šimon. An incremental isoconversional method for kinetic analysis based on the orthogonal distance regression. *Journal of Computational Chemistry*, 36(6):392–398, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dien:2014:SNU

[DDK14] Hung Dien, Charlotte M. Deane, and Bernhard Knapp. Software news and updates: Gro2mat: a package to efficiently read `gromacs` output in MATLAB. *Journal of Computational Chemistry*, 35(20):1528–1531, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dudev:2015:QCB

[DDM+15] Todor Dudev, Mike Devereux, Markus Meuwly, Carmay Lim, Jean-Philip Piquemal, and Nohad Gresh. Quantum-chemistry based calibration of the alkali metal cation series (Li^+Cs^+) for large-scale polarizable molecular mechanics/dynamics simulations. *Journal of Computational Chemistry*, 36(5):285–302, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Davie:2016:ILS

[DDP16] Stuart J. Davie, Nicodemo Di Pasquale, and Paul L. A. Popelier. Incorporation of local structure into kriging models for the prediction of atomistic properties in the water decamer. *Journal of Computational Chemistry*, 37(27):2409–2422, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeVleeschouwer:2018:CCB

[DDP+18] Freija De Vleeschouwer, Mats Denayer, Balazs Pinter, Paul Geerlings, and Frank De Proft. Characterization of chalcogen bonding interactions via an in-depth conceptual quantum chemical analysis. *Journal of Computational Chemistry*, 39 (10):557–572, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Denis:2012:IBA

[Den12] Pablo A. Denis. Interaction between alkyl radicals and single wall carbon nanotubes. *Journal of Computational Chemistry*, 33(17):1511–1516, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ding:2015:GNA

[DFF+15] Yun Ding, Ye Fang, Wei P. Feinstein, Jagannathan Ramanujam, David M. Koppelman, Juana Moreno, Michal Brylinski, and Mark Jarrell. GeauxDock: a novel approach for mixed-resolution ligand docking using a descriptor-based force field. *Journal of Computational Chemistry*, 36(27):2013–2026, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2013:PEF

[DGB+13] Likai Du, Jun Gao, Fuzhen Bi, Lili Wang, and Chengbu Liu. A polarizable ellipsoidal force field for halogen bonds. *Journal of Computational Chemistry*, 34(23):2032–2040, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DiPasquale:2014:MTS

[DGC14] Nicodemo Di Pasquale, Richard J. Gowers, and Paola Carbone. A multiple time step scheme for multiresolved models of macromolecules. *Journal of Computational Chemistry*, 35 (16):1199–1207, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeBeer:2011:MDS

[DGH+11] Stephanie B. A. De Beer, Alice GlÄttli, Johannes Hutzler, Nico P. E. Vermeulen, and Chris Oostenbrink. Molecular dynamics simulations and free energy calculations on the enzyme 4-hydroxyphenylpyruvate dioxygenase. *Journal of Computational Chemistry*, 32(10):2160–2169, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Duan:2013:TCD

[DGL+13] Yu-Ai Duan, Yun Geng, Hai-Bin Li, Jun-Ling Jin, Yong Wu, and Zhong-Min Su. Theoretical characterization and design of small molecule donor material containing naphthodithiophene central unit for efficient organic solar cells. *Journal of Computational Chemistry*, 34(19):1611–1619, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Devereux:2014:SFA

[DGPM14] Mike Devereux, Nohad Gresh, Jean-Philip Piquemal, and Markus Meuwly. A supervised fitting approach to force field parametrization with application to the SIBFA polarizable force field. *Journal of Computational Chemistry*, 35(21):1577–1591, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Douglas-Gallardo:2019:ESB

[DGSVGVM19] Oscar A. Douglas-Gallardo, David Adrian Saez, Stefan Vogt-Geisse, and Esteban Vöhringer-Martinez. Electronic structure benchmark calculations of inorganic and biochemical carboxylation reactions. *Journal of Computational Chemistry*, 40(13): 1401–1413, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dieterich:2011:CIS

[DH11] Johannes M. Dieterich and Bernd Hartke. Composition-induced structural transitions in mixed Lennard-Jones clusters: Global reparametrization and optimization. *Journal of Computational Chemistry*, 32(7):1377–1385, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dieterich:2014:GBS

[DH14] Johannes M. Dieterich and Bernd Hartke. A graph-based short-cut to low-energy structures. *Journal of Computational Chemistry*, 35(22):1618–1620, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dasgupta:2017:SGH

[DH17] Saswata Dasgupta and John M. Herbert. Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3. *Journal of Computational Chemistry*, 38(12): 869–882, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ducere:2012:CCA

[DHE+12] Jean-Marie Ducéré, Anne Hemeryck, Alain Estève, Mehdi Djafari Rouhani, Georges Landa, Philippe Ménini, Cyril Tropis, André Maisonnat, Pierre Fau, and Bruno Chaudret. A computational chemist approach to gas sensors: Modeling the response of SnO_2 to CO, O_2, and H_2O Gases. *Journal of Computational Chemistry*, 33(3):247–258, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dedachi:2011:SIB

[DHF+11] Kenichi Dedachi, Tatsuya Hirakawa, Seiya Fujita, Mahmud Tareq Hassan Khan, Ingebrigt Sylte, and Noriyuki Kurita. Specific interactions and binding free energies between thermolysin and dipeptides: Molecular simulations combined with ab initio molecular orbital and classical vibrational analysis. *Journal of Computational Chemistry*, 32(14):3047–3057, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dardouri:2013:IDE

[DHOG13] Riadh Dardouri, Héla Habli, Brahim Oujia, and Florent Xavier Gadéa. Ab Initio Diabatic energies and dipole moments of the electronic states of RbLi molecule. *Journal of Computational Chemistry*, 34(24):2091–2099, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Denis:2011:ACM

[DI11] Pablo A. Denis and Federico Iribarne. On the applicability of cluster models to study the chemical reactivity of carbon nanotubes. *Journal of Computational Chemistry*, 32(11): 2397–2403, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dillen:2015:TEF

[Dil15] Jan Dillen. The topology of the Ehrenfest force density revisited. A different perspective based on Slater-type orbitals. *Journal of Computational Chemistry*, 36(12):883–890, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dhingra:2013:HIH

[DJ13] Priyanka Dhingra and Bhyravabhotla Jayaram. A homology/ ab initio hybrid algorithm for sampling near-native protein conformations. *Journal of Computational Chemistry*, 34(22): 1925–1936, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Delgado-Jaime:2012:SNU

[DJD12] Mario Ulises Delgado-Jaime and Serena DeBeer. Software news and updates: Expedited analysis of DFT outputs: Introducing moanalyzer. *Journal of Computational Chemistry*, 33 (27):2180–2185, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dombrowsky:2018:SAA

[DJS+18] Maximilian J. Dombrowsky, Sven Jager, Benjamin Schiller, Benjamin E. Mayer, Sebastian Stammler, and Kay Hamacher.

StreaMD: Advanced analysis of molecular dynamics using R. *Journal of Computational Chemistry*, 39(21):1666–1674, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ding:2011:TPG

[DJX+11a] Zongling Ding, Jun Jiang, Huaizhong Xing, Haibo Shu, Ruibin Dong, Xiaoshuang Chen, and Wei Lu. Transport properties of graphene nanoribbon-based molecular devices. *Journal of Computational Chemistry*, 32(4):737–741, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ding:2011:FSE

[DJX+11b] Zongling Ding, Jun Jiang, Huaizhong Xing, Haibo Shu, Yan Huang, Xiaoshuang Chen, and Wei Lu. The finite-size effect on the transport properties in edge-modified graphene nanoribbon-based molecular devices. *Journal of Computational Chemistry*, 32(8):1753–1759, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeSilva:2011:EPS

[DK11] Piotr De Silva and Jacek Korchowiec. Energy partitioning scheme based on self-consistent method for subsystems: Populational space approach. *Journal of Computational Chemistry*, 32(6):1054–1064, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dahy:2019:IHU

[DK19] AbdelRahman A. Dahy and Nobuaki Koga. Imine hydrosilylation using an iron complex catalyst: a computational study. *Journal of Computational Chemistry*, 40(1):62–71, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dahanayake:2017:EES

[DKE+17] Jayangika N. Dahanayake, Chandana Kasireddy, Jonathan M. Ellis, Derek Hildebrandt, Olivia A. Hull, Joseph P. Karnes, Dylan Morlan, and Katie R. Mitchell-Koch. Evaluating electronic structure methods for accurate calculation of ^{19}F chemical shifts in fluorinated amino acids. *Journal of Computational Chemistry*, 38(30):2605–2617, November 15, 2017. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Daido:2013:NQE

[DKT13] Masashi Daido, Yukio Kawashima, and Masanori Tachikawa. Nuclear quantum effect and temperature dependency on the hydrogen-bonded structure of base pairs. *Journal of Computational Chemistry*, 34(28):2403–2411, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dauzhenka:2018:CFE

[DKV18] Taras Dauzhenka, Petras J. Kundrotas, and Ilya A. Vakser. Computational Feasibility of an Exhaustive Search of Side-Chain Conformations in Protein-Protein Docking. *Journal of Computational Chemistry*, 39(24):2012–2021, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dziubinski:2016:TIM

[DL16] Maciej Dziubiński and Bogdan Lesyng. Toward the identification of molecular cogs. *Journal of Computational Chemistry*, 37(9):848–860, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Durlak:2019:IHB

[DL19] Piotr Durlak and Zdzislaw Latajka. Investigations of the hydrogen bond in the crystals of tropolone and thiotropolone via Car–Parrinello and path integral molecular dynamics. *Journal of Computational Chemistry*, 40(4):671–687, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deLange:2017:TDD

[dLC17] Jurgens Hendrik de Lange and Ignacy Cukrowski. Toward deformation densities for intramolecular interactions without radical reference states using the fragment, atom, localized, delocalized, and interatomic (FALDI) charge density decomposition scheme. *Journal of Computational Chemistry*, 38 (13):981–997, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deLange:2018:EEE

[dLC18a] Jurgens H. de Lange and Ignacy Cukrowski. Exact and exclusive electron localization indices within QTAIM atomic basins. *Journal of Computational Chemistry*, 39(20):1517–1530, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dix:2018:WDW

[DLC18b] James Dix, Leo Lue, and Paola Carbone. Why different water models predict different structures under 2D confinement. *Journal of Computational Chemistry*, 39(25):2051–2059, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dai:2010:UGM

[DLL+10] Qi Dai, Xiaoqing Liu, Lihua Li, Yuhua Yao, Bin Han, and Lei Zhu. Using Gaussian model to improve biological sequence comparison. *Journal of Computational Chemistry*, 31(2):351–361, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2012:EFP

[DLMH12] Qi-Shi Du, Si-Yu Long, Jian-Zong Meng, and Ri-Bo Huang. Empirical formulation and parameterization of cation–π interactions for protein modeling. *Journal of Computational Chemistry*, 33(2):153–162, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dias:2011:SDP

[DLP11] R. S. Dias, P. Linse, and A. A. C. C. Pais. Stepwise disproportionation in polyelectrolyte complexes. *Journal of Computational Chemistry*, 32(12):2697–2707, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otero-de-la-Roza:2011:FAA

[dlRL11] A. Otero de-la Roza and Víctor Luaña. A fast and accurate algorithm for QTAIM integration in solids. *Journal of Computational Chemistry*, 32(2):291–305, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dias:2014:MEP

[DLSA14] Roberta P. Dias, Lin Li, Thereza A. Soares, and Emil Alexov. Modeling the electrostatic potential of asymmetric lipopolysaccharide membranes: The MEMPOT algorithm implemented in DelPhi. *Journal of Computational Chemistry*, 35(19):1418–1429, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deringer:2013:ISH

[DLSD13] Volker L. Deringer, Marck Lumeij, Ralf P. Stoffel, and Richard Dronskowski. Ab initio study of the high-temperature phase transition in crystalline GeO_2. *Journal of Computational Chemistry*, 34(27):2320–2326, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Davydova:2017:CBA

[DLT17] Elena I. Davydova, Anna S. Lisovenko, and Alexey Y. Timoshkin. Complex beryllium amidoboranes: Structures, stability, and evaluation of their potential as hydrogen storage materials. *Journal of Computational Chemistry*, 38(7):401–405, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deLange:2018:FBC

[dLvNC18a] Jurgens H. de Lange, Daniël M. E. van Niekerk, and Ignacy Cukrowski. FALDI-based criterion for and the origin of an electron density bridge with an associated (3,-1) critical point on Bader's molecular graph. *Journal of Computational Chemistry*, 39(27):2283–2299, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deLange:2018:FBD

[dLvNC18b] Jurgens H. de Lange, Daniel M. E. van Niekerk, and Ignacy Cukrowski. FALDI-based decomposition of an atomic interaction line leads to 3D representation of the multicenter nature of interactions. *Journal of Computational Chemistry*, 39(16): 973–985, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2012:ESP

[DLW12] Xiang Po Du, Veng Cheong Lo, and Yuan Xu Wang. The effect of structure and phase transformation on the mechanical properties of Re_2N and the stability of Mn_2N. *Journal of Computational Chemistry*, 33(1):18–24, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Duan:2015:UBI

[DLZ15] Rui Duan, Raudah Lazim, and Dawei Zhang. Understanding the basis of I50V-induced affinity decrease in HIV-1 protease via molecular dynamics simulations using polarized force field. *Journal of Computational Chemistry*, 36(25):1885–1892, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dolgonos:2015:SNS

[DM15] Grygoriy A. Dolgonos and Koshka Mekalka. Strain in nonclassical silicon hydrides: an insight into the “ultrastability” of sila-bi[6]prismane (Si_{18} H_{12}) cluster with the endohedrally trapped silicon atom, Si_{19} H_{12}. *Journal of Computational Chemistry*, 36(28):2095–2102, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dittner:2015:EGO

[DMAH15] Mark Dittner, Julian Müller, Hasan Metin Aktulga, and Bernd Hartke. Efficient global optimization of reactive force-field parameters. *Journal of Computational Chemistry*, 36 (20):1550–1561, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DelGaldo:2018:TAS

[DMD+18] Sara Del Galdo, Giordano Mancini, Isabella Daidone, Laura Zanetti Polzi, Andrea Amadei, and Vincenzo Barone. Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties. *Journal of Computational Chemistry*, 39(22):1747–1756, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DasGupta:2017:CAF

[DMJ17] Debarati DasGupta, Varun Mandalaparthy, and Bhyravabhotla Jayaram. A component analysis of the free energies of folding of 35 proteins: a consensus view on the thermodynamics of folding at the molecular level. *Journal of Computational*

Chemistry, 38(32):2791–2801, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeBiase:2014:MSD

[DMN14] Pablo M. De Biase, Suren Markosyan, and Sergei Noskov. Microsecond simulations of DNA and ion transport in nanopores with novel ion–ion and ion–nucleotides effective potentials. *Journal of Computational Chemistry*, 35(9):711–721, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeBiase:2015:SNU

[DMN15] Pablo M. De Biase, Suren Markosyan, and Sergei Noskov. Software news and updates: BROMOC suite: Monte Carlo/ Brownian dynamics suite for studies of ion permeation and DNA transport in biological and artificial pores with effective potentials. *Journal of Computational Chemistry*, 36(4):264–271, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dupuis:2019:MOA

[DN19] Michel Dupuis and Meghana Nallapu. Maximal orbital analysis of molecular wavefunctions. *Journal of Computational Chemistry*, 40(1):39–50, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLaPierre:2011:PSF

[DOM+11] M. De La Pierre, R. Orlando, L. Maschio, K. Doll, P. Ugliengo, and R. Dovesi. Performance of six functionals (LDA, PBE, PBESOL, B3LYP, PBE0, and WC1LYP) in the simulation of vibrational and dielectric properties of crystalline compounds. The case of forsterite Mg_2SiO_4. *Journal of Computational Chemistry*, 32(9):1775–1784, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dominikowska:2011:CDA

[DP11] Justyna Dominikowska and Marcin Palusiak. Cyclooctatetraene dianion — an artifact? *Journal of Computational Chemistry*, 32(7):1441–1448, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Drake:2015:FFD

[DP15] Justin A. Drake and B. Montgomery Pettitt. Force field-dependent solution properties of glycine oligomers. *Journal of Computational Chemistry*, 36(17):1275–1285, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dolbundalchok:2016:GCI

[DPAB16] Praphasiri Dolbundalchok, Daniel Peláez, Emad F. Aziz, and Annika Bande. Geometrical control of the interatomic Coulombic decay process in quantum dots for infrared photodetectors. *Journal of Computational Chemistry*, 37(25): 2249–2259, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dreuw:2012:CDI

[DPB+12] Andreas Dreuw, Matthias A. Polkehn, Robert Binder, Alexander Heckel, and Stefan Knippenberg. Computational design of improved two-photon active caging compounds based on nitrodibenzofuran. *Journal of Computational Chemistry*, 33(22):1797–1805, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Denning:2011:IHS

[DPNM11] Elizabeth J. Denning, U. Deva Priyakumar, Lennart Nilsson, and Alexander D. Mackerell Jr. Impact of 2'-hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM all-atom additive force field for RNA. *Journal of Computational Chemistry*, 32(9):1929–1943, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Druart:2016:PLB

[DPOS16] Karen Druart, Zoltan Palmai, Eyaz Omarjee, and Thomas Simonson. Protein:ligand binding free energies: a stringent test for computational protein design. *Journal of Computational Chemistry*, 37(4):404–415, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deb:2016:RTL

[DPSL16] Indrajit Deb, Rupak Pal, Joanna Sarzynska, and Ansuman Lahiri. Reparameterizations of the χ torsion and Lennard-

Jones σ parameters improve the conformational characteristics of modified uridines. *Journal of Computational Chemistry*, 37(17):1576–1588, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2016:HPC

[DQ16] Hongbo Du and Xianghong Qian. The hydration properties of carboxybetaine zwitterion brushes. *Journal of Computational Chemistry*, 37(10):877–885, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DaSilva:2011:CHB

[DR11] Júlio C. S. Da Silva and Willian R. Rocha. C — H bond activation of methane in aqueous solution: a hybrid quantum mechanical/effective fragment potential study. *Journal of Computational Chemistry*, 32(16):3383–3392, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Don:2014:RSS

[DR14] Charleen G. Don and Sereina Riniker. Review: Scents and sense: In silico perspectives on olfactory receptors. *Journal of Computational Chemistry*, 35(32):2279–2287, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dral:2019:MPP

[Dra19] Pavlo O. Dral. MLatom: a program package for quantum chemical research assisted by machine learning. *Journal of Computational Chemistry*, 40(26):2339–2347, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deRuiter:2013:CTI

[dRBO13] Anita de Ruiter, Stefan Boresch, and Chris Oostenbrink. Comparison of thermodynamic integration and Bennett's acceptance ratio for calculating relative protein-ligand binding free energies. *Journal of Computational Chemistry*, 34(12):1024–1034, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cuevas-Flores:2018:NIB

[dRCFGRB18] Ma del Refugio Cuevas-Flores, Marco Antonio Garcia-Revilla, and Massimiliano Bartolomei. Noncovalent interactions between cisplatin and graphene prototypes. *Journal of Computational Chemistry*, 39(2):71–80, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dryzun:2014:CSM

[Dry14] Chaim Dryzun. Continuous symmetry measures for complex symmetry group. *Journal of Computational Chemistry*, 35(9): 748–755, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deglmann:2012:TCR

[DS12a] Peter Deglmann and Stephan Schenk. Thermodynamics of chemical reactions with COSMO-RS: the extreme case of charge separation or recombination. *Journal of Computational Chemistry*, 33(14):1304–1320, May 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deshmukh:2012:TSE

[DS12b] Milind M. Deshmukh and Shigeyoshi Sakaki. Two-step evaluation of binding energy and potential energy surface of van der Waals complexes. *Journal of Computational Chemistry*, 33(6):617–628, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dash:2015:GGS

[DS15] Tirtharaj Dash and Prabhat K. Sahu. Gradient gravitational search: an efficient metaheuristic algorithm for global optimization. *Journal of Computational Chemistry*, 36(14):1060–1068, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

dosSantos:2013:PAF

[dSAdSL13] Marcus V. P. dos Santos, Eduardo C. Aguiar, João Bosco P. da Silva, and Ricardo L. Longo. PICVib: an accurate, fast, and simple procedure to investigate selected vibrational modes at high theoretical levels. *Journal of Computational Chemistry*, 34(8):611–621, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dressler:2019:ERL

[DSAS19] Christian Dreßler, Arne Scherrer, Paul Ahlert, and Daniel Sebastiani. Efficient representation of the linear density-density response function. *Journal of Computational Chemistry*, 40 (31):2712–2721, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Daoudi:2019:ESO

[DSB+19] Syrine Daoudi, Abderrahmane Semmeq, Michael Badawi, Xavier Assfeld, Youssef Arfaoui, and Mariachiara Pastore. Electronic structure and optical properties of isolated and TiO_2-grafted free base porphyrins for water oxidation: a challenging test case for DFT and TD-DFT. *Journal of Computational Chemistry*, 40(29):2530–2538, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeJong:2011:DEC

[DSD+11] Djurre H. De Jong, Lars V. Schäfer, Alex H. De Vries, Siewert J. Marrink, Herman J. C. Berendsen, and Helmut Grubmüller. Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. *Journal of Computational Chemistry*, 32(9):1919–1928, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

daSilva:2010:DSF

[dSDdAR10] Júlio C. S. da Silva, Roberta P. Dias, Wagner B. de Almeida, and Willian R. Rocha. DFT study of the full catalytic cycle for the propene hydroformylation catalyzed by a heterobimetallic $HPt(SnCl_3)(PH_3)_2$ model catalyst. *Journal of Computational Chemistry*, 31(10):1986–2000, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

daSilva:2017:TSS

[dSdLBNB17] Vitor H. Menezes da Silva, Ana Paula de Lima Batista, Oscar Navarro, and Ataualpa A. C. Braga. Theoretical study on selectivity trends in (*N*-heterocyclic carbene)-Pd catalyzed Mizoroki–Heck reactions: Exploring density functionals methods and molecular models. *Journal of Computational Chemistry*, 38(28):2371–2377, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

daSilva:2012:DFT

[dSdS12a] Luís Pinto da Silva and Joaquim C. G. Esteves da Silva. Density functional theory study of 1,2-dioxetanone decomposition in condensed phase. *Journal of Computational Chemistry*, 33(26):2118–2123, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [RSLML12] and reply [dSdS12b].

daSilva:2012:LER

[dSdS12b] Luís Pinto da Silva and Joaquim C. G. Esteves da Silva. Letters to the editor: Response to "Comment on density functional theory study of 1,2-dioxetanone decomposition in condensed phase". *Journal of Computational Chemistry*, 33(26):2127–2130, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [dSdS12a, RSLML12].

Dutagaci:2017:HDG

[DSF17] Bercem Dutagaci, Maryam Sayadi, and Michael Feig. Heterogeneous dielectric generalized Born model with a van der Waals term provides improved association energetics of membrane-embedded transmembrane helices. *Journal of Computational Chemistry*, 38(16):1308–1320, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

daSilva:2019:IIA

[dSH19] Natieli Alves da Silva and Roberto Luiz Andrade Haiduke. Infrared intensity analysis of hydroxyl stretching modes in carboxylic acid dimers by means of the charge–charge flux–dipole flux model. *Journal of Computational Chemistry*, 40 (28):2482–2490, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dyduch:2018:ECS

[DSHLM18] Karol Dyduch, Monika Srebro-Hooper, Bun Yeoul Lee, and Artur Michalak. Exploring the conformational space of cobalt(III)-salen catalyst for CO_2 /epoxide copolymerization: Effect of quaternary ammonium salts on preference of alternative isomers. *Journal of Computational Chemistry*, 39(23): 1854–1867, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dohm:2017:SNU

[DSK17] Sebastian Dohm, Eckhard Spohr, and Martin Korth. Software news and updates: Developing adaptive QM/MM computer simulations for electrochemistry. *Journal of Computational Chemistry*, 38(1):51–58, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeLaLande:2011:SDA

[DSM+11] Aurelien De La Lande, Dennis R. Salahub, Jacques Maddaluno, Anthony Scemama, Julien Pilme, Olivier Parisel, Helene Gerard, Michel Caffarel, and Jean-Philip Piquemal. Spin-driven activation of dioxygen in various metalloenzymes and their inspired models. *Journal of Computational Chemistry*, 32(6):1178–1182, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Delcey:2019:ECL

[DSV+19] Mickael G. Delcey, Lasse Kragh Sørensen, Morgane Vacher, Rafael C. Couto, and Marcus Lundberg. Efficient calculations of a large number of highly excited states for multiconfigurational wavefunctions. *Journal of Computational Chemistry*, 40(19):1789–1799, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deSouza:2016:RCS

[dSVdM+16] Miguel A. F. de Souza, Elizete Ventura, Silmar A. do Monte, José M. Riveros, and Ricardo L. Longo. Revisiting the concept of the (a)synchronicity of Diels–Alder reactions based on the dynamics of quasiclassical trajectories. *Journal of Computational Chemistry*, 37(8):701–711, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2011:MMS

[DSX+11] Juan Du, Huijun Sun, Lili Xi, Jiazhong Li, Ying Yang, Huanxiang Liu, and Xiaojun Yao. Molecular modeling study of checkpoint kinase 1 inhibitors by multiple docking strategies and prime/MM–GBSA calculation. *Journal of Computational Chemistry*, 32(13):2800–2809, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dreux:2019:ESE

[DT19] Katelyn M. Dreux and Gregory S. Tschumper. Examination of the structures, energetics, and vibrational frequencies of small sulfur-containing prototypical dimers, $(H_2\ S)_2$ and H_2 O/ H_2 S. *Journal of Computational Chemistry*, 40(1):229–236, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deVaca:2016:SNU

[dVAG16] Israel Cabeza de Vaca, Sandra Acebes, and Victor Guallar. Software news and updates: Ecoupling server: a tool to compute and analyze electronic couplings. *Journal of Computational Chemistry*, 37(18):1740–1745, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DiDomizio:2014:SNU

[DVVP14] Alessandro Di Domizio, Alessandro Vitriolo, Giulio Vistoli, and Alessandro Pedretti. Software news and updates: SPILLO–PBSS: Detecting hidden binding sites within protein 3D-structures through a flexible structure-based approach. *Journal of Computational Chemistry*, 35(27):2005–2017, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deVries:2017:FAG

[dVZ17] Sjoerd J. de Vries and Martin Zacharias. Fast and accurate grid representations for atom-based docking with partner flexibility. *Journal of Computational Chemistry*, 38(17):1538–1546, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dieterich:2017:SNU

[DWC17] Johannes M. Dieterich, William C. Witt, and Emily A. Carter. Software news and updates: libKEDF: an accelerated library of kinetic energy density functionals. *Journal of Computational Chemistry*, 38(17):1552–1559, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dai:2011:IPS

[DWL11] Qi Dai, Li Wu, and Lihua Li. Improving protein structural class prediction using novel combined sequence information and predicted secondary structural features. *Journal of Computational Chemistry*, 32(16):3393–3398, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deng:2017:EMC

[DWR17] Shi Deng, Qiantao Wang, and Pengyu Ren. Estimating and modeling charge transfer from the SAPT induction energy. *Journal of Computational Chemistry*, 38(26):2222–2231, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dang:2017:FSW

[DWZ+17] Jing-Shuang Dang, Wei-Wei Wang, Jia-Jia Zheng, Shigeru Nagase, and Xiang Zhao. Formation of Stone–Wales edge: Multistep reconstruction and growth mechanisms of zigzag nanographene. *Journal of Computational Chemistry*, 38(26): 2241–2247, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Du:2010:SBQ

[DXL+10] Juan Du, Lili Xi, Beilei Lei, Jing Lu, Jiazhong Li, Huanxiang Liu, and Xiaojun Yao. Structure-based quantitative structure-activity relationship studies of checkpoint kinase 1 inhibitors. *Journal of Computational Chemistry*, 31(15):2783–2793, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dryzun:2011:QSC

[DZA11] Chaim Dryzun, Amir Zait, and David Avnir. Quantitative symmetry and chirality — a fast computational algorithm for large structures: Proteins, macromolecules, nanotubes, and unit cells. *Journal of Computational Chemistry*, 32(12):2526–2538, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dlugosz:2011:BDS

[DZT11] Maciej Długosz, Paweł Zieliński, and Joanna Trylska. Brownian dynamics simulations on CPU and GPU with BD_BOX. *Journal of Computational Chemistry*, 32(12):2734–2744, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2012:FPC

[EB12] Robert A. Evarestov and Andrei V. Bandura. First-principles calculations on the four phases of $BaTiO_3$. *Journal of Computational Chemistry*, 33(11):1123–1130, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2018:IRA

[EB18] Robert A. Evarestov and Andrei V. Bandura. Infrared and Raman active vibrational modes in MoS_2-based nanotubes: Symmetry analysis and first-principles calculations. *Journal of Computational Chemistry*, 39(26):2163–2172, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2013:BBN

[EBK13] Robert A. Evarestov, Andrei V. Bandura, and Dmitrii D. Kuruch. $BaTiO_3$-based nanolayers and nanotubes: First-principles calculations. *Journal of Computational Chemistry*, 34(3):175–186, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2017:FPM

[EBPK17a] Robert A. Evarestov, Andrei V. Bandura, Vitaly V. Porsev, and Alexey V. Kovalenko. First-principles modeling of hafnia-based nanotubes. *Journal of Computational Chemistry*, 38(24):2088–2099, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2017:PSE

[EBPK17b] Robert A. Evarestov, Andrei V. Bandura, Vitaly V. Porsev, and Alexey V. Kovalenko. Phonon spectra, electronic, and thermodynamic properties of WS_2 nanotubes. *Journal of Computational Chemistry*, 38(30):2581–2593, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Erba:2017:NRE

[ECZWD17] Alessandro Erba, Dominique Caglioti, Claudio Marcelo Zicovich-Wilson, and Roberto Dovesi. Nuclear-relaxed elastic and piezoelectric constants of materials: Computational aspects of two quantum-mechanical approaches. *Journal of*

Computational Chemistry, 38(5):257–264, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eller:2015:CAE

[ED15] Joshua J. Eller and Karen Downey. Computational assessment of electron density in metallo-organic nickel pincer complexes for formation of P C bonds. *Journal of Computational Chemistry*, 36(26):1947–1953, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Elias:2018:MIS

[EdOdS18] Thiago Castilho Elias, Humberto César Brandão de Oliveira, and Nelson José Freitas da Silveira. MB-Isoster: a software for bioisosterism simulation. *Journal of Computational Chemistry*, 39(29):2481–2487, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehara:2013:CII

[EFAC13] Masahiro Ehara, Ryoichi Fukuda, Carlo Adamo, and Ilaria Ciofini. Chemically intuitive indices for charge-transfer excitation based on SAC-CI and TD-DFT calculations. *Journal of Computational Chemistry*, 34(29):2498–2501, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Edel:2016:IFP

[EFB16] Klara Edel, Reinhold F. Fink, and Holger F. Bettinger. Isomerization and fragmentation pathways of 1,2-azaborine. *Journal of Computational Chemistry*, 37(1):110–116, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Erba:2013:ADS

[EFOD13] Alessandro Erba, Matteo Ferrabone, Roberto Orlando, and Roberto Dovesi. Accurate dynamical structure factors from ab initio lattice dynamics: the case of crystalline silicon. *Journal of Computational Chemistry*, 34(5):346–354, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehara:2016:PCS

[EFS16] Masahiro Ehara, Ryoichi Fukuda, and Thomas Sommerfeld. Projected CAP/SAC-CI method with smooth Voronoi potential for calculating resonance states. *Journal of Computational Chemistry*, 37(2):242–249, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Elenewski:2013:CPC

[EH13] Justin E. Elenewski and John C. Hackett. Cytochrome P450 compound I in the plane wave pseudopotential framework: GGA electronic and geometric structure of thiolate-ligated iron(IV)–oxo porphyrin. *Journal of Computational Chemistry*, 34(19):1647–1660, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

El-Hamdi:2016:CAB

[EHSPT16] Majid El-Hamdi, Miquel Solà, Jordi Poater, and Alexey Y. Timoshkin. Complexes of adamantane-based group 13 Lewis acids and superacids: Bonding analysis and thermodynamics of hydrogen splitting. *Journal of Computational Chemistry*, 37(15):1355–1362, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

El-Hamdi:2019:HSP

[EHT19] Majid El-Hamdi and Alexey Y. Timoshkin. Hydrogen splitting by pyramidalized 13–15 donor–acceptor cryptands: a computational study. *Journal of Computational Chemistry*, 40(21):1892–1901, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eisenberg:2013:RTG

[EJ13] Azaria Solomon Eisenberg and Laura J. Juszczak. Relating Trp-Glu dipeptide fluorescence to molecular conformation: the role of the discrete chi 1 and chi 2 angles. *Journal of Computational Chemistry*, 34(18):1549–1560, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eilmes:2015:SIT

[EK15] Andrzej Eilmes and Piotr Kubisiak. Stability of ion triplets in ionic liquid/lithium salt solutions: Insights from implicit and explicit solvent models and molecular dynamics simulations.

Journal of Computational Chemistry, 36(10):751–762, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehlert:2017:QBS

[EK17] Christopher Ehlert and Tillmann Klamroth. The quest for best suited references for configuration interaction singles calculations of core excited states. *Journal of Computational Chemistry*, 38(2):116–126, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ekesan:2014:TPE

[EKH14] Solen Ekesan, Seyit Kale, and Judith Herzfeld. Transferable pseudoclassical electrons for aufbau of atomic ions. *Journal of Computational Chemistry*, 35(15):1159–1164, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Elking:2016:TAF

[Elk16] Dennis M. Elking. Torque and atomic forces for Cartesian tensor atomic multipoles with an application to crystal unit cell optimization. *Journal of Computational Chemistry*, 37(22):2067–2080, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Emamian:2019:ENP

[ELKE19] Saeedreza Emamian, Tian Lu, Holger Kruse, and Hamidreza Emamian. Exploring nature and predicting strength of hydrogen bonds: a correlation analysis between atoms-in-molecules descriptors, binding energies, and energy components of symmetry-adapted perturbation theory. *Journal of Computational Chemistry*, 40(32):2868–2881, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eng:2019:GDT

[ELP19] Julien Eng, Beth A. Laidlaw, and Thomas J. Penfold. On the geometry dependence of tuned-range separated hybrid functionals. *Journal of Computational Chemistry*, 40(25):2191–2199, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Esser:2017:AFP

[EMD17] Marc Esser, Stefan Maintz, and Richard Dronskowski. Automated first-principles mapping for phase-change materials. *Journal of Computational Chemistry*, 38(9):620–628, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

ElKhoury:2017:IES

[ENKK+17] Léa El Khoury, Sehr Naseem-Khan, Karolina Kwapien, Zeina Hobaika, Richard G. Maroun, Jean-Philip Piquemal, and Nohad Gresh. Importance of explicit smeared lone-pairs in anisotropic polarizable molecular mechanics. Torture track angular tests for exchange-repulsion and charge transfer contributions. *Journal of Computational Chemistry*, 38(22): 1897–1920, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eriksen:2011:CPP

[EOA+11] Janus J. Eriksen, Jógvan Magnus H. Olsen, Kestutis Aidas, Hans Ågren, Kurt V. Mikkelsen, and Jacob Kongsted. Computational protocols for prediction of solute NMR relative chemical shifts. A case study of L-tryptophan in aqueous solution. *Journal of Computational Chemistry*, 32(13):2853–2864, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Erlebach:2016:TCA

[EOO+16] Andreas Erlebach, Timm Ott, Christoph Otzen, Stephanie Schubert, Justyna Czaplewska, Ulrich S. Schubert, and Marek Sierka. Thermodynamic compatibility of actives encapsulated into PEG-PLA nanoparticles: In silico predictions and experimental verification. *Journal of Computational Chemistry*, 37(24):2220–2227, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eastman:2010:ENI

[EP10] Peter Eastman and Vijay S. Pande. Efficient nonbonded interactions for molecular dynamics on a graphics processing unit. *Journal of Computational Chemistry*, 31(6):1268–1272, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Erba:2012:EEM

[EP12] Alessandro Erba and Cesare Pisani. Evaluation of the electron momentum density of crystalline systems from ab initio linear combination of atomic orbitals calculations. *Journal of Computational Chemistry*, 33(8):822–831, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2015:SCE

[EP15] Robert A. Evarestov and Andrej I. Panin. Symmetry classification of electron and phonon states in TiO_2-based nanowires and nanotubes. *Journal of Computational Chemistry*, 36(13): 957–969, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Elking:2010:AFG

[EPD+10] Dennis M. Elking, Lalith Perera, Robert Duke, Thomas Darden, and Lee G. Pedersen. Atomic forces for geometry-dependent point multipole and Gaussian multipole models. *Journal of Computational Chemistry*, 31(15):2702–2713, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Elking:2011:FFM

[EPD+11] Dennis M. Elking, Lalith Perera, Robert Duke, Thomas Darden, and Lee G. Pedersen. A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. *Journal of Computational Chemistry*, 32(15):3283–3295, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

ElHage:2013:CAM

[EPH+13] Krystel El Hage, Jean-Philip Piquemal, Zeina Hobaika, Richard G. Maroun, and Nohad Gresh. Could an anisotropic molecular mechanics/dynamics potential account for sigma hole effects in the complexes of halogenated compounds? *Journal of Computational Chemistry*, 34(13):1125–1135, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

ElHage:2015:CJL

[EPH+15] Krystel El Hage, Jean-Philip Piquemal, Zeina Hobaika, Richard G. Maroun, and Nohad Gresh. Could the "Janus-like" properties of the halobenzene CX bond (X = Cl, Br) be leveraged to enhance molecular recognition? *Journal of Computational Chemistry*, 36(4):210–221, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Edorh:2018:IUE

[ER18] Semeho Prince A. Edorh and Stéphane Redon. Incremental update of electrostatic interactions in adaptively restrained particle simulations. *Journal of Computational Chemistry*, 39(20):1455–1469, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ellingson:2013:SNU

[ESB13] Sally R. Ellingson, Jeremy C. Smith, and Jerome Baudry. Software news and updates: VinaMPI: Facilitating multiple receptor high-throughput virtual docking on high-performance computers. *Journal of Computational Chemistry*, 34(25):2212–2221, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eberhardt:2018:USA

[ESD18] Jérôme Eberhardt, Roland H. Stote, and Annick Dejaegere. Unrolr: Structural analysis of protein conformations using stochastic proximity embedding. *Journal of Computational Chemistry*, 39(30):2551–2557, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eriksen:2012:IES

[ESM+12] Janus J. Eriksen, Stephan P. A. Sauer, Kurt V. Mikkelsen, Hans J. Aa. Jensen, and Jacob Kongsted. On the importance of excited state dynamic response electron correlation in polarizable embedding methods. *Journal of Computational Chemistry*, 33(25):2012–2022, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ellis:2017:CDC

[ETLS17] Christopher R. Ellis, Cheng-Chieh Tsai, Fang-Yu Lin, and Jana Shen. Conformational dynamics of cathepsin D and binding to a small-molecule BACE1 inhibitor. *Journal of Computational Chemistry*, 38(15):1260–1269, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eskandari:2014:HHI

[EV14] Kiamars Eskandari and Christian Van Alsenoy. Hydrogen–hydrogen interaction in planar biphenyl: a theoretical study based on the interacting quantum atoms and Hirshfeld atomic energy partitioning methods. *Journal of Computational Chemistry*, 35(26):1883–1889, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eidi:2018:CVF

[EVR18] Mohammadreza Eidi, Mohsen Vafaee, and Mitra Rooein. Complementary version of fermion coupled coherent states method and Gram–Schmidt algorithm: Theory and applications for electronic states of H_2 and H_2^+. *Journal of Computational Chemistry*, 39(11):679–684, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Escorcia:2018:MDS

[EvRC+18] Andrés M. Escorcia, Jeaphianne P. M. van Rijn, Gui-Juan Cheng, Patrick Schrepfer, Thomas B. Brück, and Walter Thiel. Molecular dynamics study of taxadiene synthase catalysis. *Journal of Computational Chemistry*, 39(19):1215–1225, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Epifanovsky:2013:SNU

[EWK+13] Evgeny Epifanovsky, Michael Wormit, Tomasz Kuś, Arie Landau, Dmitry Zuev, Kirill Khistyaev, Prashant Manohar, Ilya Kaliman, Andreas Dreuw, and Anna I. Krylov. Software news and updates: New implementation of high-level correlated methods using a general block tensor library for high-performance electronic structure calculations. *Journal of Computational Chemistry*, 34(26):2293–2309, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fredin:2018:SCI

[FA18] Lisa A. Fredin and Thomas C. Allison. Semiempirical configuration interaction calculations for ru-centered dyes*. *Jour-*

nal of Computational Chemistry*, 39(19):1259–1266, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farhat:2015:ICG

[FAA15] Ayman Farhat and Saleh N. Abdul-Al. Ab initio calculations of the ground and excited states of the ZrN molecule including spin-orbit effects. *Journal of Computational Chemistry*, 36 (16):1252–1258, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farley:2018:SMN

[FAS+18] Christopher Farley, Amit Aggarwal, Sunaina Singh, Aaron Dolor, Philip To, Alexander Falber, Maxwell Crossley, and Charles Michael Drain. A Structural Model of Nitro-Porphyrin Dyes Based on Spectroscopy and Density Functional Theory. *Journal of Computational Chemistry*, 39(18): 1129–1142, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferro:2010:AQC

[FB10] Noel Ferro and Thomas Bredow. Assessment of quantum-chemical methods for electronic properties and geometry of signaling biomolecules. *Journal of Computational Chemistry*, 31(5):1063–1079, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandez:2012:AER

[FB12] Israel Fernández and F. Matthias Bickelhaupt. Alder-ene reaction: Aromaticity and activation-strain analysis. *Journal of Computational Chemistry*, 33(5):509–516, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandez:2014:OER

[FB14a] Israel Fernández and F. Matthias Bickelhaupt. Origin of the "endo rule" in Diels–Alder reactions. *Journal of Computational Chemistry*, 35(5):371–376, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Futera:2014:RMR

[FB14b] Zdeněk Futera and Jaroslav V. Burda. Reaction mechanism of Ru(II) piano-stool complexes: Umbrella sampling QM/MM

MD study. *Journal of Computational Chemistry*, 35(19):1446–1456, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Forti:2011:CCI

[FBEM11] Flavio Forti, Leonardo Boechi, Dario A. Estrin, and Marcelo A. Marti. Comparing and combining implicit ligand sampling with multiple steered molecular dynamics to study ligand migration processes in heme proteins. *Journal of Computational Chemistry*, 32(10):2219–2231, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fletcher:2019:VMP

[FBKD19] Graham D. Fletcher, Colleen Bertoni, Murat Keçeli, and Michael D'Mello. Valence: A massively parallel implementation of the variational subspace valence bond method. *Journal of Computational Chemistry*, 40(17):1664–1673, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fonseca:2018:CFP

[FBvdB18] Rasmus Fonseca, Dominik Budday, and Henry van den Bedem. Collision-free Poisson motion planning in ultra high-dimensional molecular conformation spaces. *Journal of Computational Chemistry*, 39(12):711–720, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Felberg:2017:POS

[FBY+17] Lisa E. Felberg, David H. Brookes, Eng-Hui Yap, Elizabeth Jurrus, Nathan A. Baker, and Teresa Head-Gordon. PB-AM: an open-source, fully analytical linear Poisson–Boltzmann solver. *Journal of Computational Chemistry*, 38(15):1275–1282, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandez:2016:IBA

[FC16] Israel Fernández and Fernando P. Cossío. Interplay between aromaticity and strain in double group transfer reactions to 1,2-benzyne. *Journal of Computational Chemistry*, 37(14):1265–1273, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Frishberg:2018:CSE

[FC18] Carol Frishberg and Leon Cohen. Contracted Schrödinger equation in quantum phase-space. *Journal of Computational Chemistry*, 39(17):1068–1075, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Francisco:2017:MAI

[FCCP17] Evelio Francisco, Daniel Menéndez Crespo, Aurora Costales, and Ángel Martín Pendás. A multipolar approach to the interatomic covalent interaction energy. *Journal of Computational Chemistry*, 38(11):816–829, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferrari:2010:IPS

[FCD10] Anna Maria Ferrari, Bartolomeo Civalleri, and Roberto Dovesi. Ab initio periodic study of the conformational behavior of glycine helical homopeptides. *Journal of Computational Chemistry*, 31(8):1777–1784, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fogolari:2015:AAL

[FCE15] Federico Fogolari, Alessandra Corazza, and Gennaro Esposito. Accuracy assessment of the linear Poisson–Boltzmann equation and reparametrization of the OBC generalized Born model for nucleic acids and nucleic acid–protein complexes. *Journal of Computational Chemistry*, 36(9):585–596, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fan:2010:NDB

[FCL+10] Feng Fan, Jiagao Cheng, Zhong Li, Xiaoyong Xu, and Xuhong Qian. Novel dimer based descriptors with solvational computation for QSAR study of oxadiazoylbenzoyl-ureas as novel insect-growth regulators. *Journal of Computational Chemistry*, 31(3):586–591, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferro-Costas:2012:QBE

[FCOGM12] David Ferro-Costas, Nicolás Otero, Ana M. Graña, and Ricardo A. Mosquera. A QTAIM-based energy partitioning for understanding the physical origin of conformational preferences: Application to the Z effect in $O = C - X - R$ and related units. *Journal of Computational Chemistry*, 33(32): 2533–2543, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferro-Costas:2014:EEB

[FCPJM14] David Ferro-Costas, Ignacio Pérez-Juste, and Ricardo A. Mosquera. Electronegativity estimator built on QTAIM-based domains of the bond electron density. *Journal of Computational Chemistry*, 35(13):978–985, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fu:2014:MIN

[FCW+14] Bing Fu, Li Chen, Feifei Wang, Yiqun Xie, and Xiang Ye. Melting of icosahedral nickel clusters under hydrostatic pressure. *Journal of Computational Chemistry*, 35(31):2231–2238, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Falklof:2013:MPA

[FD13] Olle Falklöf and Bo Durbeej. Modeling of phytochrome absorption spectra. *Journal of Computational Chemistry*, 34 (16):1363–1374, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Falklof:2014:DBK

[FD14] Olle Falklöf and Bo Durbeej. Distinguishing between keto–enol and acid–base forms of firefly oxyluciferin through calculation of excited-state equilibrium constants. *Journal of Computational Chemistry*, 35(30):2184–2194, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fumanal:2016:DES

[FD16] Maria Fumanal and Chantal Daniel. Description of excited states in $[Re(Imidazole)(CO)_3 (Phen)]^+$ including solvent and spin-orbit coupling effects: Density functional theory versus multiconfigurational wavefunction approach. *Journal of Computational Chemistry*, 37(27):2454–2466, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farren-Dai:2018:CSP

[FDCJG18] Marco Farren-Dai, Stanley Cameron, Michel B. Johnson, and Khashayar Ghandi. Crystal Structure and Properties of Imidazo-Pyridine Ionic Liquids. *Journal of Computational Chemistry*, 39(18):1149–1157, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Freibert:2019:ESO

[FDH19] Antonia Freibert, Johannnes M. Dieterich, and Bernd Hartke. Exploring self-organization of molecular tether molecules on a gold surface by global structure optimization. *Journal of Computational Chemistry*, 40(22):1978–1989, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fukuda:2014:EPS

[FE14] Ryoichi Fukuda and Masahiro Ehara. Efficiency of perturbation-selection and its orbital dependence in the SAC–CI calculations for valence excitations of medium-size molecules. *Journal of Computational Chemistry*, 35(30):2163–2176, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferreira:2017:TCP

[FED17] Lizé-Mari Ferreira, Alan Eaby, and Jan Dillen. The topology of the Coulomb potential density. A comparison with the electron density, the virial energy density, and the Ehrenfest force density. *Journal of Computational Chemistry*, 38(32): 2784–2790, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feldkamp:2010:CDN

[Fel10] Udo Feldkamp. CANADA: Designing nucleic acid sequences for nanobiotechnology applications. *Journal of Computational Chemistry*, 31(3):660–663, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferenczy:2013:CWFb

[Fer13a] György G. Ferenczy. Calculation of wave-functions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. II. Application of the local basis equation. *Journal of Computational Chemistry*, 34(10):862–869, April

5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferenczy:2013:CWFa

[Fer13b] György G. Ferenczy. Calculation of wave-functions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. Part I. Application of the Huzinaga equation. *Journal of Computational Chemistry*, 34(10):854–861, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ferguson:2017:BBA

[Fer17] Andrew L. Ferguson. BayesWHAM: a Bayesian approach for free energy estimation, reweighting, and uncertainty quantification in the weighted histogram analysis method. *Journal of Computational Chemistry*, 38(18):1583–1605, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farrokhpour:2011:TSV

[FF11] Hossein Farrokhpour and Fariman Fathi. Theoretical study of valance photoelectron spectra of hypoxanthine, xanthine, and caffeine using direct symmetry-adapted cluster/configuration interaction methodology. *Journal of Computational Chemistry*, 32(11):2479–2491, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fracchia:2014:MLQ

[FFA14] Francesco Fracchia, Claudia Filippi, and Claudio Amovilli. Multi-level quantum Monte Carlo wave functions for complex reactions: the decomposition of α-hydroxy-dimethylnitrosamine. *Journal of Computational Chemistry*, 35(1):30–38, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fedichev:2011:CEM

[FGM11] P. O. Fedichev, E. G. Getmantsev, and L. I. Menshikov. $O(N \log N)$ continuous electrostatics method for fast calculation of solvation energies of biomolecules. *Journal of Computational Chemistry*, 32(7):1368–1376, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fumanal:2019:ESR

[FHG+19] Maria Fumanal, Yu Harabuchi, Etienne Gindensperger, Satoshi Maeda, and Chantal Daniel. Excited-state reactivity of $[Mn(im)(CO)_3\ (phen)]^+$: a structural exploration. *Journal of Computational Chemistry*, 40(1):72–81, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujimoto:2012:POE

[FHK+12] Hirofumi Fujimoto, Mariko Higuchi, Manabu Koike, Hirotaka Ode, Miroslav Pinak, Juraj Kotulic Bunta, Toshiyuki Nemoto, Takashi Sakudoh, Naoko Honda, Hideaki Maekawa, Kimiaki Saito, and Kozo Tsuchida. A possible overestimation of the effect of acetylation on lysine residues in KQ mutant analysis. *Journal of Computational Chemistry*, 33(3): 239–246, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fenley:2015:FCP

[FHMB15] Marcia O. Fenley, Robert C. Harris, Travis Mackoy, and Alexander H. Boschitsch. Features of CPB: a Poisson–Boltzmann solver that uses an adaptive cartesian grid. *Journal of Computational Chemistry*, 36(4):235–243, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fihey:2015:SDP

[FHT+15] Arnaud Fihey, Christian Hettich, Jérémy Touzeau, François Maurel, Aurélie Perrier, Christof Köhler, Bálint Aradi, and Thomas Frauenheim. SCC–DFTB parameters for simulating hybrid gold-thiolates compounds. *Journal of Computational Chemistry*, 36(27):2075–2087, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fink:2011:PCA

[FHW+11] Florian Fink, Jochen Hochrein, Vincent Wolowski, Rainer Merkl, and Wolfram Gronwald. PROCOS: Computational analysis of protein–protein complexes. *Journal of Computational Chemistry*, 32(12):2575–2586, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fias:2018:RFS

[FHZA+18] Stijn Fias, Farnaz Heidar-Zadeh, James S. M. Anderson, Paul W. Ayers, and Robert G. Parr. A reference-free stockholder partitioning method based on the force on electrons. *Journal of Computational Chemistry*, 39(17):1044–1050, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fuhrer:2015:IPR

[FL15] Timothy J. Fuhrer and Angel M. Lambert. Isolated pentagon rule violating endohedral metallofullerenes explained using the Hückel rule: a statistical mechanical study of the C_{84} Isomeric Set. *Journal of Computational Chemistry*, 36 (3):146–150, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fu:2011:AAS

[FLM11] Zheng Fu, Xue Li, and Kenneth M. Merz Jr. Accurate assessment of the strain energy in a protein-bound drug using QM/MM X-ray refinement and converged quantum chemistry. *Journal of Computational Chemistry*, 32(12):2587–2597, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feng:2010:SDP

[FM10] Jianwen A. Feng and Garland R. Marshall. SKATE: a docking program that decouples systematic sampling from scoring. *Journal of Computational Chemistry*, 31(14):2540–2554, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Foster:2012:BTF

[FMG12] Theresa J. Foster, Alexander D. MacKerell Jr., and Olgun Guvench. Balancing target flexibility and target denaturation in computational fragment-based inhibitor discovery. *Journal of Computational Chemistry*, 33(23):1880–1891, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farrokhpour:2011:IPE

[FMNC11] Hossein Farrokhpour, Zainab Mombeini, Mansoor Namazian, and Michelle L. Coote. Intermolecular potential energy surface for CS_2 dimer. *Journal of Computational Chemistry*, 32 (5):797–809, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farrell:2012:SNU

[FN12] Damien Farrell and Jens Erik Nielsen. Software news and updates: DataPipeline: Automated importing and fitting of large amounts of biophysical data. *Journal of Computational Chemistry*, 33(29):2357–2362, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Foroutan-Nejad:2011:DRC

[FNSF+11] Cina Foroutan-Nejad, Shant Shahbazian, Ferran Feixas, Parviz Rashidi-Ranjbar, and Miquel Solà. A dissected ring current model for assessing magnetic aromaticity: a general approach for both organic and inorganic rings. *Journal of Computational Chemistry*, 32(11):2422–2431, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fomin:2011:CDL

[Fom11] Eduard S. Fomin. Consideration of data load time on modern processors for the Verlet table and linked-cell algorithms. *Journal of Computational Chemistry*, 32(7):1386–1399, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fomin:2013:MDS

[Fom13] Yu. D. Fomin. Molecular dynamics simulation of benzene in graphite and amorphous carbon slit pores. *Journal of Computational Chemistry*, 34(30):2615–2624, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fletcher:2017:FTP

[FP17a] Timothy L. Fletcher and Paul L. A. Popelier. FFLUX: Transferability of polarizable machine-learned electrostatics in peptide chains. *Journal of Computational Chemistry*, 38(13): 1005–1014, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fletcher:2017:TAA

[FP17b] Timothy L. Fletcher and Paul L. A. Popelier. Toward amino acid typing for proteins in FFLUX. *Journal of Computational Chemistry*, 38(6):336–345, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Futera:2012:BPS

[FPB12] Zdeněk Futera, James A. Platts, and Jaroslav V. Burda. Binding of piano-stool Ru(II) complexes to DNA; QM/MM study. *Journal of Computational Chemistry*, 33(26):2092–2101, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujimoto:2019:DDF

[FPH+19] Kazushi Fujimoto, Rajadeep Singh Payal, Tomonori Hattori, Wataru Shinoda, Masayuki Nakagaki, Shigeyoshi Sakaki, and Susumu Okazaki. Development of dissociative force field for all-atomistic molecular dynamics calculation of fracture of polymers. *Journal of Computational Chemistry*, 40(29):2571–2576, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Forni:2014:HBB

[FPRS14] Alessandra Forni, Stefano Pieraccini, Stefano Rendine, and Maurizio Sironi. Halogen bonds with benzene: an assessment of DFT functionals. *Journal of Computational Chemistry*, 35 (5):386–394, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Franchini:2013:BFC

[FPV13] Mirko Franchini, Pierre Herman Theodoor Philipsen, and Lucas Visscher. The Becke Fuzzy Cells Integration Scheme in the Amsterdam Density Functional Program Suite. *Journal of Computational Chemistry*, 34(21):1819–1827, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fraenkel:2015:ISL

[Fra15] Dan Fraenkel. Ion strength limit of computed excess functions based on the linearized Poisson–Boltzmann equation. *Journal of Computational Chemistry*, 36(31):2302–2316, December 5,

2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [Fra16].

Fraenkel:2016:ECI

[Fra16] Dan Fraenkel. Erratum: Corrigendum: Ion strength limit of computed excess functions based on the linearized Poisson–Boltzmann equation. *Journal of Computational Chemistry*, 37(32):2816, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [Fra15].

Fernandes:2018:MVP

[FRC18] Henrique S. Fernandes, Maria J. Ramos, and Nuno M. F. S. A. Cerqueira. molUP: a VMD plugin to handle QM and ONIOM calculations using the Gaussian software. *Journal of Computational Chemistry*, 39(19):1344–1353, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fuhrmann:2010:NLG

[FRLN10] Jan Fuhrmann, Alexander Rurainski, Hans-Peter Lenhof, and Dirk Neumann. A new Lamarckian genetic algorithm for flexible ligand-receptor docking. *Journal of Computational Chemistry*, 31(9):1911–1918, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandes:2015:QSL

[FRN15] Kyle D. Fernandes, C. Alicia Renison, and Kevin J. Naidoo. Quantum supercharger library: Hyper-parallelism of the Hartree–Fock method. *Journal of Computational Chemistry*, 36(18):1399–1409, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Farahani:2014:RTS

[FRSA14] Pooria Farahani, Daniel Roca-Sanjuán, and Francesco Aquilante. Review: a two-scale approach to electron correlation in multiconfigurational perturbation theory. *Journal of Computational Chemistry*, 35(22):1609–1617, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fu:2014:SNU

[FSC+14] Biao Fu, Aleksandr B. Sahakyan, Carlo Camilloni, Gian Gaetano Tartaglia, Emanuele Paci, Amedeo Caflisch, Michele

Vendruscolo, and Andrea Cavalli. Software news and updates: ALMOST: an all atom molecular simulation toolkit for protein structure determination. *Journal of Computational Chemistry*, 35(14):1101–1105, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Furmanchuk:2018:PSC

[FSD+18] Al'ona Furmanchuk, James E. Saal, Jeff W. Doak, Gregory B. Olson, Alok Choudhary, and Ankit Agrawal. Prediction of Seebeck coefficient for compounds without restriction to fixed stoichiometry: a machine learning approach. *Journal of Computational Chemistry*, 39(4):191–202, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fought:2017:STE

[FSSW17] Ellie L. Fought, Vaibhav Sundriyal, Masha Sosonkina, and Theresa L. Windus. Saving time and energy with oversubscription and semi-direct Møller–Plesset second order perturbation methods. *Journal of Computational Chemistry*, 38(11): 830–841, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fought:2019:IES

[FSSW19] Ellie L. Fought, Vaibhav Sundriyal, Masha Sosonkina, and Theresa L. Windus. Improving efficiency of semi-direct Møller–Plesset second-order perturbation methods through oversubscription on multiple nodes. *Journal of Computational Chemistry*, 40(24):2146–2157, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fomin:2015:BBC

[FTR15] Yury D. Fomin, Elena N. Tsiok, and Valentin N. Ryzhov. The behavior of benzene confined in a single wall carbon nanotube. *Journal of Computational Chemistry*, 36(12):901–906, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Flick:2012:MLB

[FTW12] Johannes Flick, Frank Tristram, and Wolfgang Wenzel. Modeling loop backbone flexibility in receptor-ligand docking simulations. *Journal of Computational Chemistry*, 33(31):2504–

2515, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fias:2010:MDI

[FVB10] Stijn Fias, Sofie Van Damme, and Patrick Bultinck. Multidimensionality of delocalization indices and nucleus-independent chemical shifts in polycyclic aromatic hydrocarbons II: Proof of further nonlocality. *Journal of Computational Chemistry*, 31(12):2286–2293, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fertitta:2014:AMA

[FVP14] Edoardo Fertitta, Elena Voloshina, and Beate Paulus. Adsorption of multivalent alkylthiols on Au(111) surface: Insights from DFT. *Journal of Computational Chemistry*, 35 (3):204–213, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandez:2014:COA

[FWB14] Israel Fernández, Lando P. Wolters, and F. Matthias Bickelhaupt. Controlling the oxidative addition of aryl halides to Au(I). *Journal of Computational Chemistry*, 35(29):2140–2145, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feng:2018:TST

[FWS+18] Songyan Feng, Keke Wen, Yubing Si, Xugeng Guo, and Jinglai Zhang. Theoretical studies on thermally activated delayed fluorescence mechanism of a series of organic light-emitting diodes emitters comprising 2,7-diphenylamino-9,9-dimethylacridine as electron donor. *Journal of Computational Chemistry*, 39(31):2601–2606, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feng:2013:MGM

[FXC+13] Xin Feng, Kelin Xia, Zhan Chen, Yiying Tong, and Guo-Wei Wei. Multiscale geometric modeling of macromolecules II: Lagrangian representation. *Journal of Computational Chemistry*, 34(24):2100–2120, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fan:2015:DDS

[FZL+15] Guo-Liang Fan, Xiao-Yan Zhang, Yan-Ling Liu, Yi Nang, and Hui Wang. DSPMP: Discriminating secretory proteins of malaria parasite by hybridizing different descriptors of Chou's pseudo amino acid patterns. *Journal of Computational Chemistry*, 36(31):2317–2327, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fu:2019:CDZ

[FZL+19] Cen-Feng Fu, Ruiqi Zhang, Qiquan Luo, Xingxing Li, and Jinlong Yang. Construction of direct Z-Scheme photocatalysts for overall water splitting using two-dimensional van der Waals heterojunctions of metal dichalcogenides. *Journal of Computational Chemistry*, 40(9):980–987, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Faraggi:2012:SXI

[FZY+12] Eshel Faraggi, Tuo Zhang, Yuedong Yang, Lukasz Kurgan, and Yaoqi Zhou. SPINE X: Improving protein secondary structure prediction by multistep learning coupled with prediction of solvent accessible surface area and backbone torsion angles. *Journal of Computational Chemistry*, 33(3):259–267, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glushkov:2012:OCM

[GA12] V. N. Glushkov and X. Assfeld. On orthogonality constrained multiple core-hole states and optimized effective potential method. *Journal of Computational Chemistry*, 33(26):2058–2066, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glushkov:2014:MSF

[GA14] Vitaly N. Glushkov and Xavier Assfeld. Multireference space without first solving the configuration interaction problem. *Journal of Computational Chemistry*, 35(4):313–323, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grabarek:2018:IES

[GA18] Dawid Grabarek and Tadeusz Andruniów. Initial excited-state relaxation of locked retinal protonated Schiff base chromophore. An insight from coupled cluster and multireference perturbation theory calculations. *Journal of Computational Chemistry*, 39(22):1720–1727, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gordeev:2019:SNC

[GA19] Evgeniy G. Gordeev and Valentine P. Ananikov. Switching the nature of catalytic centers in Pd/ NHC systems by solvent effect driven non-classical R-NHC Coupling. *Journal of Computational Chemistry*, 40(1):191–199, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galano:2013:CMA

[GAI13] Annia Galano and Juan Raúl Alvarez-Idaboy. A computational methodology for accurate predictions of rate constants in solution: Application to the assessment of primary antioxidant activity. *Journal of Computational Chemistry*, 34(28): 2430–2445, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galano:2014:KRM

[GAI14] Annia Galano and Juan Raúl Alvarez-Idaboy. Kinetics of radical-molecule reactions in aqueous solution: a benchmark study of the performance of density functional methods. *Journal of Computational Chemistry*, 35(28):2019–2026, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gruden:2017:BDF

[GAJ+17] Maja Gruden, Ljubica Andjeklović, Akkarapattiakal Kuriappan Jissy, Stepan Stepanović, Matija Zlatar, Qiang Cui, and Marcus Elstner. Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. *Journal of Computational Chemistry*, 38(25): 2171–2185, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grande-Aztatzi:2014:SES

[GAMAC+14] Rafael Grande-Aztatzi, Paulina R. Martínez-Alanis, José Luis Cabellos, Edison Osorio, Ana Martínez, and Gabriel Merino. Structural evolution of small gold clusters doped by one and two boron atoms. *Journal of Computational Chemistry*, 35

(32):2288–2296, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garberoglio:2012:SNU

[Gar12] Giovanni Garberoglio. Software news and updates: OBGMX: a Web-based generator of GROMACS topologies for molecular and periodic systems using the universal force field. *Journal of Computational Chemistry*, 33(27):2204–2208, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gavrish:2012:AER

[Gav12] Sergey P. Gavrish. Approximate expressions and the relationship between pyramidalization (out-of-plane deformation) characteristics of trigonal centers. *Journal of Computational Chemistry*, 33(27):2173–2179, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gumerov:2012:HAF

[GBFD12] Nail A. Gumerov, Konstantin Berlin, David Fushman, and Ramani Duraiswami. A hierarchical algorithm for fast Debye summation with applications to small angle scattering. *Journal of Computational Chemistry*, 33(25):1981–1996, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gutsev:2019:HDM

[GBG+19] G. L. Gutsev, K. V. Bozhenko, L. G. Gutsev, A. N. Utenyshev, and S. M. Aldoshin. Hydrogenation of 3 d-metal oxide clusters: Effects on the structure and magnetic properties. *Journal of Computational Chemistry*, 40(3):562–571, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gutsev:2016:SPI

[GBGR16] Gennady L. Gutsev, Kalayu G. Belay, Lavrenty G. Gutsev, and Bala R. Ramachandran. Structure and properties of iron oxide clusters: From Fe_6 to Fe_6O_{20} and from Fe_7 to Fe_7O_{24}. *Journal of Computational Chemistry*, 37(28):2527–2536, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ganesan:2011:SDE

[GBL+11] Narayan Ganesan, Brad A. Bauer, Timothy R. Lucas, Sandeep Patel, and Michela Taufer. Structural, dynamic, and electrostatic properties of fully hydrated DMPC bilayers from molecular dynamics simulations accelerated with graphical processing units (GPUs). *Journal of Computational Chemistry*, 32(14):2958–2973, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia:2019:EST

[GBPCC19] Juan Sanz García, Martial Boggio-Pasqua, Ilaria Ciofini, and Marco Campetella. Excited state tracking during the relaxation of coordination compounds. *Journal of Computational Chemistry*, 40(14):1420–1428, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gross:2017:MAI

[GBS+17] Lynn Groß, Marc Philipp Bahlke, Torben Steenbock, Christian Klinke, and Carmen Herrmann. Modeling adsorbate-induced property changes of carbon nanotubes. *Journal of Computational Chemistry*, 38(12):861–868, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grebner:2011:ETS

[GBSE11] Christoph Grebner, Johannes Becker, Svetlana Stepanenko, and Bernd Engels. Efficiency of tabu-search-based conformational search algorithms. *Journal of Computational Chemistry*, 32(10):2245–2253, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghillemijn:2011:SCH

[GBVA11] Dieter Ghillemijn, Patrick Bultinck, Dimitri Van Neck, and Paul W. Ayers. A self-consistent Hirshfeld method for the atom in the molecule based on minimization of information loss. *Journal of Computational Chemistry*, 32(8):1561–1567, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grebner:2014:SNU

[GBW+14] Christoph Grebner, Johannes Becker, Daniel Weber, Daniel Bellinger, Maxim Tafipolski, Charlotte Brückner, and Bernd

Engels. Software news and updates: CAST: a new program package for the accurate characterization of large and flexible molecular systems. *Journal of Computational Chemistry*, 35(24):1801–1807, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gupta:2011:NDI

[GC11] Rini Gupta and Amalendu Chandra. Nonideality in diffusion of ionic and neutral solutes and hydrogen bond dynamics in dimethyl sulfoxide–chloroform mixtures of varying composition. *Journal of Computational Chemistry*, 32(12):2679–2689, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghorai:2018:PSL

[GC18] Sankar Ghorai and Pinaki Chaudhury. Predicting stability limits for pure and doped dicationic noble gas clusters undergoing Coulomb explosion: a parallel tempering based study. *Journal of Computational Chemistry*, 39(14):827–838, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gramatica:2014:SNU

[GCC14] Paola Gramatica, Stefano Cassani, and Nicola Chirico. Software news and updates: QSARINS-chem: Insubria datasets and new QSAR/QSPR models for environmental pollutants in QSARINS. *Journal of Computational Chemistry*, 35(13): 1036–1044, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghosh:2015:RSS

[GCCM15] Anirban Ghosh, Rajat K. Chaudhuri, Sudip Chattopadhyay, and Uttam Sinha Mahapatra. Relativistic state-specific multireference perturbation theory incorporating improved virtual orbitals: Application to the ground state single-bond dissociation. *Journal of Computational Chemistry*, 36(26): 1954–1972, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gramatica:2013:SNU

[GCP+13] Paola Gramatica, Nicola Chirico, Ester Papa, Stefano Cassani, and Simona Kovarich. Software news and updates: QSARINS: a new software for the development, analysis, and validation of QSAR MLR models. *Journal of Computational Chemistry*, 34(24):2121–2132, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gotz:2014:EIQ

[GCW14] Andreas W. Götz, Matthew A. Clark, and Ross C. Walker. An extensible interface for QM/MM molecular dynamics simulations with AMBER. *Journal of Computational Chemistry*, 35(2):95–108, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gong:2016:ACD

[GCW16] Xiping Gong, Zhenhua Chen, and Wei Wu. The application of Cholesky decomposition in valence bond calculation. *Journal of Computational Chemistry*, 37(23):2157–2162, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2015:EPC

[GCWS15] David Z. Gao, Filippo Federici Canova, Matthew B. Watkins, and Alexander L. Shluger. Efficient parametrization of complex molecule–surface force fields. *Journal of Computational Chemistry*, 36(16):1187–1195, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gillessen:2010:CSI

[GD10] Michael Gilleßen and Richard Dronskowski. A combinatorial study of inverse Heusler alloys by first-principles computational methods. *Journal of Computational Chemistry*, 31(3): 612–619, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2017:IFP

[GDV17] Cen Gao, Jeremy Desaphy, and Michal Vieth. Are induced fit protein conformational changes caused by ligand-binding predictable? A molecular dynamics investigation. *Journal of Computational Chemistry*, 38(15):1229–1237, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grimme:2011:EDF

[GEG11] Stefan Grimme, Stephan Ehrlich, and Lars Goerigk. Effect of the damping function in dispersion corrected density functional theory. *Journal of Computational Chemistry*, 32(7): 1456–1465, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gresh:2014:PMM

[GEP+14] Nohad Gresh, Krystel El Hage, David Perahia, Jean-Philip Piquemal, Catherine Berthomieu, and Dorothée Berthomieu. Polarizable molecular mechanics studies of Cu(I)/Zn(II) superoxide dismutase: Bimetallic binding site and structured waters. *Journal of Computational Chemistry*, 35(29):2096–2106, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goldstein:2011:NHA

[GFG11] Moshe Goldstein, Erick Fredj, and R. Benny Gerber. A new hybrid algorithm for finding the lowest minima of potential surfaces: Approach and application to peptides. *Journal of Computational Chemistry*, 32(9):1785–1800, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Godey:2018:EGT

[GFGS18] François Godey, Alexandre Fleury, Aziz Ghoufi, and Armand Soldera. The extent of the glass transition from molecular simulation revealing an overcrank effect. *Journal of Computational Chemistry*, 39(5):255–261, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghasemi:2017:RDS

[GFPSD17] Fahimeh Ghasemi, Afshin Fassihi, Horacio Pérez-Sánchez, and Alireza Mehri Dehnavi. The role of different sampling methods in improving biological activity prediction using deep belief network. *Journal of Computational Chemistry*, 38(4): 195–203, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galvez:2010:TST

[GG10] Jesús Gálvez and Antonio Guirado. A theoretical study of topomerization of imine systems: Inversion, rotation or mixed mechanisms? *Journal of Computational Chemistry*, 31(3): 520–531, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gotze:2012:BHN

[GGM+12] Jan P. Götze, Claudio Greco, Roland Mitrić, Vlasta Bonačić-Koutecký, and Peter Saalfrank. BLUF hydrogen network dynamics and UV/Vis spectra: a combined molecular dynamics and quantum chemical study. *Journal of Computational Chemistry*, 33(28):2233–2242, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Georgieva:2010:QCM

[GH10] Polina Georgieva and Fahmi Himo. Quantum chemical modeling of enzymatic reactions: the case of histone lysine methyltransferase. *Journal of Computational Chemistry*, 31(8):1707–1714, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gross:2016:LED

[GH16a] Lynn Groß and Carmen Herrmann. Local electric dipole moments: a generalized approach. *Journal of Computational Chemistry*, 37(25):2260–2265, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gross:2016:SNU

[GH16b] Lynn Groß and Carmen Herrmann. Software news and updates: GenLocDip: a generalized program to calculate and visualize local electric dipole moments. *Journal of Computational Chemistry*, 37(25):2324–2334, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2012:AFE

[GHK12] Cen Gao, J. Martin Herold, and Dmitri Kireev. Assessment of free energy predictors for ligand binding to a methyllysine histone code reader. *Journal of Computational Chemistry*, 33(6):659–665, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gamez:2017:ADF

[GHL17] José A. Gámez, Markus Hölscher, and Walter Leitner. On the applicability of density functional theory to manganese-based complexes with catalytic activity toward water oxidation. *Journal of Computational Chemistry*, 38(20):1747–1751, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goh:2017:RDL

[GHV17] Garrett B. Goh, Nathan O. Hodas, and Abhinav Vishnu. Review: Deep learning for computational chemistry. *Journal of Computational Chemistry*, 38(16):1291–1307, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gilbert:2011:TOG

[Gil11] Thomas M. Gilbert. Testing the ONIOM G2R3 model against donor–acceptor dissociation energies of group 13–15 complexes: Accuracy comparable to CCSD(T)/aug-CC-pVTZ at a fraction of the resource cost. *Journal of Computational Chemistry*, 32(8):1493–1499, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Jacas:2014:SNU

[GJMPAM+14] César R. García-Jacas, Yovani Marrero-Ponce, Liesner Acevedo-Martínez, Stephen J. Barigye, José R. Valdés-Martiní, and Ernesto Contreras-Torres. Software news and updates: QuBiLS–MIDAS: a parallel free-software for molecular descriptors computation based on multilinear algebraic maps. *Journal of Computational Chemistry*, 35(18):1395–1409, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gertych:2010:IPS

[GK10] Artur Gertych and Jacek Koput. Ab initio prediction of the structure and vibration-rotation spectroscopic properties of Na_2OH and K_2OH. *Journal of Computational Chemistry*, 31 (7):1542–1549, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galstyan:2015:CPV

[GK15a] Gegham Galstyan and Ernst-Walter Knapp. Computing pK_A values of hexa-aqua transition metal complexes. *Journal of Computational Chemistry*, 36(2):69–78, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gunera:2015:FBS

[GK15b] Jakub Gunera and Peter Kolb. Fragment-based similarity searching with infinite color space. *Journal of Computational Chemistry*, 36(21):1597–1608, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Getmanskii:2019:MDS

[GKB+19] Iliya V. Getmanskii, Vitaliy V. Koval, Alexander I. Boldyrev, Ruslan M. Minyaev, and Vladimir I. Minkin. Molecular dynamics study of a new metastable allotropic crystalline form of gallium-supertetrahedral gallium. *Journal of Computational Chemistry*, 40(20):1861–1865, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gavane:2019:THT

[GKJ+19] Vivek Gavane, Shruti Koulgi, Vinod Jani, Mallikarjunachari V. N. Uppuladinne, Uddhavesh Sonavane, and Rajendra Joshi. TANGO: a high through-put conformation generation and semiempirical method-based optimization tool for ligand molecules. *Journal of Computational Chemistry*, 40(7):900–909, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gramatica:2013:LER

[GKR13] Paola Gramatica, Simona Kovarich, and Partha Pratim Roy. Letters to the editor: Reply to the comment of S. Rayne on "QSAR model reproducibility and applicability: a case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzo-)triazoles". *Journal of Computational Chemistry*, 34(20):1796, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [RKG11, Ray13].

Glukhova:2014:MFB

[GKSS14] Olga E. Glukhova, Anna S. Kolesnikova, Michael M. Slepchenkov, and Vladislav V. Shunaev. Moving of fullerene between potential wells in the external icosahedral shell. *Journal of Computational Chemistry*, 35(17):1270–1277, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghosh:2013:EFP

[GKV+13] Debashree Ghosh, Dmytro Kosenkov, Vitalii Vanovschi, Joanna Flick, Ilya Kaliman, Yihan Shao, Andrew T. B. Gilbert, Anna I. Krylov, and Lyudmila V. Slipchenko. Effective fragment potential method in Q-CHEM: a guide for users and developers. *Journal of Computational Chemistry*, 34(12):1060–1070, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gagnon:2016:FCD

[GLB16] Jessica K. Gagnon, Sean M. Law, and Charles L. Brooks III. Flexible CDOCKER: Development and application of a pseudo-explicit structure-based docking method within CHARMM. *Journal of Computational Chemistry*, 37(8):753–762, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gan:2016:SIR

[GLF16] Li-Hua Gan, Dan Lei, and Patrick W. Fowler. Structural interconnections and the role of heptagonal rings in endohedral trimetallic nitride template fullerenes. *Journal of Computational Chemistry*, 37(20):1907–1913, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gillet:2017:TER

[GLM+17] Natacha Gillet, Bernard Lévy, Vicent Moliner, Isabelle Demachy, and Aurélien de la Lande. Theoretical estimation of redox potential of biological quinone cofactors. *Journal of Computational Chemistry*, 38(18):1612–1621, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glendening:2013:ENN

[GLW13a] Eric D. Glendening, Clark R. Landis, and Frank Weinhold. Erratum: NBO 6.0: Natural bond orbital analysis program. *Journal of Computational Chemistry*, 34(24):2134, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GLW13b].

Glendening:2013:SNU

[GLW13b] Eric D. Glendening, Clark R. Landis, and Frank Weinhold. Software news and updates: NBO 6.0: Natural bond orbital analysis program. *Journal of Computational Chemistry*, 34(16):1429–1437, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [GLW13a].

Glendening:2019:NNV

[GLW19] Eric D. Glendening, Clark R. Landis, and Frank Weinhold. NBO 7.0: New vistas in localized and delocalized chemical bonding theory. *Journal of Computational Chemistry*, 40(25): 2234–2241, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2017:TSC

[GLZ17] Jingyuan Gao, Wenliang Li, and Jingping Zhang. Theoretical simulation of CO_2 capture in organic cage impregnated with polyoxometalates. *Journal of Computational Chemistry*, 38 (9):612–619, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghazouani:2017:SCV

[GM17] Anis Ghazouani and Jalel M'halla. Simple computing of the viscosity of water–dioxane mixtures, according to a fluctuating SPC/E-I_h interstitial model. *Journal of Computational Chemistry*, 38(22):1952–1965, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galindo-Murillo:2016:MDM

[GMASBF16] Rodrigo Galindo-Murillo, Luis Enrique Aguilar-Suárez, and Joaquín Barroso-Flores. A mixed DFT-MD methodology for the *in silico* development of drug releasing macrocycles. Calix and thia-calix[N]arenes as carriers for Bosutinib and Sorafenib. *Journal of Computational Chemistry*, 37(10):940–946, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gatti:2018:EDS

[GMBM18] Carlo Gatti, Giovanni Macetti, Russell J. Boyd, and Chérif F. Matta. An Electron Density Source-Function Study of DNA Base Pairs in Their Neutral and Ionized Ground States$^+$. *Journal of Computational Chemistry*, 39(18):1112–1128, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guo:2016:DQT

[GMBX+16] Huan Guo, Alejandro Morales-Bayuelo, Tianlv Xu, Roya Momen, Lingling Wang, Ping Yang, Steven R. Kirk, and Samantha Jenkins. Distinguishing and quantifying the torquoselectivity in competitive ring-opening reactions using the stress tensor and QTAIM. *Journal of Computational Chemistry*, 37 (31):2722–2733, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gotz:2010:MEE

[GMG+10] Kathrin Götz, Florian Meier, Carlo Gatti, Asbjörn M. Burow, Marek Sierka, Joachim Sauer, and Martin Kaupp. Modeling environmental effects on charge density distributions in polar organometallics: Validation of embedded cluster models for the methyl lithium crystal. *Journal of Computational Chemistry*, 31(14):2568–2576, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ginex:2016:DVH

[GMMH+16] Tiziana Ginex, Jordi Muñoz-Muriedas, Enric Herrero, Enric Gibert, Pietro Cozzini, and F. J. Luque. Development and validation of hydrophobic molecular fields derived from the quantum mechanical IEF/PCM-MST solvation models in 3D-QSAR. *Journal of Computational Chemistry*, 37(13):1147–1162, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Graf:2016:FEC

[GMO16] Michael M. H. Graf, Manuela Maurer, and Chris Oostenbrink. Free-energy calculations of residue mutations in a tripeptide using various methods to overcome inefficient sampling. *Journal of Computational Chemistry*, 37(29):2597–2605, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghysels:2012:CNM

[GMPB12] An Ghysels, Benjamin T. Miller, Frank C. Pickard IV, and Bernard R. Brooks. Comparing normal modes across different models and scales: Hessian reduction versus coarse-graining. *Journal of Computational Chemistry*, 33(28):2250–2275, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gapsys:2015:SNU

[GMSdG15] Vytautas Gapsys, Servaas Michielssens, Daniel Seeliger, and Bert L. de Groot. Software news and updates: `pmx`: Automated protein structure and topology generation for alchemical perturbations. *Journal of Computational Chemistry*, 36 (5):348–354, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garay:2014:FAC

[GMSV14] Pablo G. Garay, Osvaldo A. Martin, Harold A. Scheraga, and Jorge A. Vila. Factors affecting the computation of the ^{13}C shielding in disaccharides. *Journal of Computational Chemistry*, 35(25):1854–1864, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gfeller:2012:EMM

[GMZ12] David Gfeller, Olivier Michielin, and Vincent Zoete. Expanding molecular modeling and design tools to non-natural sidechains. *Journal of Computational Chemistry*, 33(18): 1525–1535, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galabov:2018:HEH

[GNC+18] Boris Galabov, Valia Nikolova, Diana Cheshmedzhieva, Boriana Hadjieva, and Henry F. Schaefer III. Hyperconjugative effects in π-hydrogen bonding: Theory and experiment. *Journal of Computational Chemistry*, 39(10):527–534, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gonzalez-Navarrete:2012:EFD

[GNDA+12] Patricio González-Navarrete, Luis R. Domingo, Juan Andrés, Slawomir Berski, and Bernard Silvi. Electronic fluxes during Diels–Alder reactions involving 1,2-benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. *Journal of Computational Chemistry*, 33(30):2400–2411, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gonzalez-Navarrete:2010:DFT

[GNGCA10] P. González-Navarrete, L. Gracia, M. Calatayud, and J. AndréS. Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. *Journal of Computational Chemistry*, 31(13):2493–2501, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goodarzi:2018:ESP

[GNI18] Moein Goodarzi, Fariba Nazari, and Francesc Illas. Electronic and structural properties of Li_n @Be_2 B_8 (n = 1-14) and Li_n @Be_2 B_{36} (n = 1-21) nanoflakes shed light on possible anode materials for Li-based batteries. *Journal of Computational Chemistry*, 39(22):1795–1805, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garate:2013:FED

[GO13] Jose Antonio Garate and Chris Oostenbrink. Free-energy differences between states with different conformational ensembles. *Journal of Computational Chemistry*, 34(16):1398–1408, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gonnet:2012:PVL

[Gon12] Pedro Gonnet. Pairwise Verlet lists: Combining cell lists and Verlet lists to improve memory locality and parallelism. *Journal of Computational Chemistry*, 33(1):76–81, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Granucci:2011:GCI

[GP11a] Giovanni Granucci and Maurizio Persico. Gradients for configuration interaction energies with spin-orbit coupling in a semiempirical framework. *Journal of Computational Chemistry*, 32(12):2690–2696, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gruber:2011:SBL

[GP11b] Christian C. Gruber and Jürgen Pleiss. Systematic benchmarking of large molecular dynamics simulations employing GROMACS on massive multiprocessing facilities. *Journal of Computational Chemistry*, 32(4):600–606, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gereben:2012:RCC

[GP12] Orsolya Gereben and László Pusztai. RMC_POT: a computer code for reverse Monte Carlo modeling the structure of disordered systems containing molecules of arbitrary complexity. *Journal of Computational Chemistry*, 33(29):2285–2291, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gresh:2016:CZM

[GPdC+16] Nohad Gresh, David Perahia, Benoit de Courcy, Johanna Foret, Céline Roux, Lea El-Khoury, Jean-Philip Piquemal, and Laurent Salmon. Complexes of a Zn-metalloenzyme binding site with hydroxamate-containing ligands. A case for detailed benchmarkings of polarizable molecular mechanics/dynamics potentials when the experimental binding structure is unknown. *Journal of Computational Chemistry*, 37(32):2770–2782, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grebner:2013:PGT

[GPE13] Christoph Grebner, Lukas P. Pason, and Bernd Engels. PathOpt — a global transition state search approach: Outline of algorithm. *Journal of Computational Chemistry*, 34(21):1810–1818, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gregori-Puigjane:2011:IMC

[GPGSM11] Elisabet Gregori-Puigjané, Rut Garriga-Sust, and Jordi Mestres. Indexing molecules with chemical graph identifiers. *Journal of Computational Chemistry*, 32(12):2638–2646, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [Ihl12] and response [GPGSM12].

Gregori-Puigjane:2012:LER

[GPGSM12] Elisabet Gregori-Puigjané, Rut Garriga-Sust, and Jordi Mestres. Letters to the editor: Response to the comment by Wolf Ihlenfeldt on the paper “Indexing molecules with chemical graph identifiers”. *Journal of Computational Chemistry*, 33(2):238, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GPGSM11, Ihl12].

Gusarov:2012:ETS

[GPK12] Sergey Gusarov, Bhalchandra S. Pujari, and Andriy Kovalenko. Efficient treatment of solvation shells in 3D molecular theory of solvation. *Journal of Computational Chemistry*, 33(17):1478–1494, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghara:2016:SSN

[GPK+16] Manas Ghara, Sudip Pan, Anand Kumar, Gabriel Merino, and Pratim K. Chattaraj. Structure, stability, and nature of bonding in carbon monoxide bound EX3+ complexes (E = group 14 element; X = H, F, Cl, Br, I). *Journal of Computational Chemistry*, 37(24):2202–2211, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghersi:2017:CQR

[GPM17] Dario Ghersi, Abhishek Parakh, and Mihaly Mezei. Comparison of a quantum random number generator with pseudorandom number generators for their use in molecular Monte Carlo simulations. *Journal of Computational Chemistry*, 38 (31):2713–2720, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Geppert:2010:PPD

[GPS10] Tim Geppert, Ewgenij Proschak, and Gisbert Schneider. Protein-protein docking by shape-complementarity and property matching. *Journal of Computational Chemistry*, 31(9): 1919–1928, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Genheden:2010:HOS

[GR10a] Samuel Genheden and Ulf Ryde. How to obtain statistically converged MM/GBSA results. *Journal of Computational Chemistry*, 31(4):837–846, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grudinin:2010:PMM

[GR10b] Sergei Grudinin and Stephane Redon. Practical modeling of molecular systems with symmetries. *Journal of Computational Chemistry*, 31(9):1799–1814, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Genheden:2011:CDI

[GR11] Samuel Genheden and Ulf Ryde. A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. *Journal of Computational Chemistry*, 32(2):187–195, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grajciar:2015:LMI

[Gra15] Lukáš Grajciar. Low-memory iterative density fitting. *Journal of Computational Chemistry*, 36(20):1521–1535, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grabowski:2018:TFT

[Gra18] Sławomir J. Grabowski. Two faces of triel bonds in boron trihalide complexes. *Journal of Computational Chemistry*, 39 (9):472–480, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Risueno:2014:SPP

[GRARO+14] Pablo García-Risueño, Joseba Alberdi-Rodriguez, Micael J. T. Oliveira, Xavier Andrade, Michael Pippig, Javier Muguerza, Agustin Arruabarrena, and Angel Rubio. A survey of the parallel performance and accuracy of Poisson solvers for electronic structure calculations. *Journal of Computational Chemistry*, 35(6):427–444, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gonzalez:2012:SRI

[GRCL12] Marta González, Roi Álvarez Rodríguez, Maria Magdalena Cid, and Carlos Silva López. A stepwise retro-imino-ene as a key step in the mechanism of allene formation via the Crabbé acetylene homologation. *Journal of Computational Chemistry*, 33(13):1236–1239, May 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Giri:2010:BAS

[GRD+10] Santanab Giri, Debesh Ranjan Roy, Soma Duley, Arindam Chakraborty, Ramakrishnan Parthasarathi, Munusamy Elango, Ramadoss Vijayaraj, Venkatesan Subramanian, Rafael Islas, Gabriel Merino, and Pratim Kumar Chattaraj. Bonding, aromaticity, and structure of trigonal dianion metal clusters.

Journal of Computational Chemistry, 31(9):1815–1821, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Risueno:2011:EEC

[GREA11] Pablo García-Risueño, Pablo Echenique, and J. L. Alonso. Exact and efficient calculation of Lagrange multipliers in biological polymers with constrained bond lengths and bond angles: Proteins and nucleic acids as example cases. *Journal of Computational Chemistry*, 32(14):3039–3046, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grigoryan:2013:AFE

[Gri13] Gevorg Grigoryan. Absolute free energies of biomolecules from unperturbed ensembles. *Journal of Computational Chemistry*, 34(31):2726–2741, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guo:2011:PPF

[GRL+11] Jianxiu Guo, Nini Rao, Guangxiong Liu, Yong Yang, and Gang Wang. Predicting protein folding rates using the concept of Chou's pseudo amino acid composition. *Journal of Computational Chemistry*, 32(8):1612–1617, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). This article has been retracted: see [GRL+12].

Guo:2012:RPP

[GRL+12] Jianxiu Guo, Nini Rao, Guangxiong Liu, Yong Yang, and Gang Wang. Retracted: Predicting protein folding rates using the concept of Chou's pseudo amino acid composition. *Journal of Computational Chemistry*, 33(32):2614, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GRL+11]. From the publisher: "The retraction has been agreed due to significant overlap with respect to another article, 'Predicting Protein Folding Rate from Amino Acid Sequence,' published in Progress in Biochemistry and Biophysics (2010, **37**, 1331) and authored by a subset of the present authors.".

Garcia-Rates:2019:EIA

[GRN19] Miquel Garcia-Ratés and Frank Neese. Efficient implementation of the analytical second derivatives of Hartree–Fock and hybrid DFT energies within the framework of the conductor-like polarizable continuum model. *Journal of Computational Chemistry*, 40(20):1816–1828, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Geppert:2012:VSC

[GRP+12] Tim Geppert, Felix Reisen, Max Pillong, Volker Hähnke, Yusuf Tanrikulu, Christian P. Koch, Anna Maria Perna, Tatiana Batista Perez, Petra Schneider, and Gisbert Schneider. Virtual screening for compounds that mimic protein–protein interface epitopes. *Journal of Computational Chemistry*, 33 (5):573–579, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Genheden:2015:BAA

[GRS15] Samuel Genheden, Ulf Ryde, and Pär Söderhjelm. Binding affinities by alchemical perturbation using QM/ MM with a large QM system and polarizable MM model. *Journal of Computational Chemistry*, 36(28):2114–2124, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grigoropoulos:2011:SEP

[GS11] Alexios Grigoropoulos and Robert K. Szilagyi. In silico evaluation of proposed biosynthetic pathways for the unique dithiolate ligand of the H-cluster of [FeFe]-hydrogenase. *Journal of Computational Chemistry*, 32(15):3194–3206, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gomes:2012:SNU

[GS12] Thiago C. F. Gomes and Munir S. Skaf. Software news and updates: Cellulose-Builder: a toolkit for building crystalline structures of cellulose. *Journal of Computational Chemistry*, 33(14):1338–1346, May 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gaillard:2014:PDM

[GS14] Thomas Gaillard and Thomas Simonson. Pairwise decomposition of an MMGBSA energy function for computational protein design. *Journal of Computational Chemistry*, 35(18): 1371–1387, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galvelis:2015:RSE

[GS15] Raimondas Galvelis and Yuji Sugita. Replica state exchange metadynamics for improving the convergence of free energy estimates. *Journal of Computational Chemistry*, 36(19):1446–1455, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Galvelis:2016:FAW

[GS16] Raimondas Galvelis and Yuji Sugita. The following articles were published in past issues of the *Journal of Computational Chemistry*: Replica state exchange metadynamics for improving the convergence of free energy estimates. *Journal of Computational Chemistry*, 37(6), March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gadre:2018:P

[GS18] Shridhar R. Gadre and C. H. Suresh. Preface. *Journal of Computational Chemistry*, 39(9):457, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grauffel:2010:FFP

[GSD10] Cédric Grauffel, Roland H. Stote, and Annick Dejaegere. Force field parameters for the simulation of modified histone tails. *Journal of Computational Chemistry*, 31(13):2434–2451, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Sosa:2010:DEI

[GSHM10] Alfonso T. García-Sosa, Csaba Hetényi, and Uko Maran. Drug efficiency indices for improvement of molecular docking scoring functions. *Journal of Computational Chemistry*, 31(1):174–184, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gapurenko:2015:GCG

[GSMM15] Olga A. Gapurenko, Andrey G. Starikov, Ruslan M. Minyaev, and Vladimir I. Minkin. Germanium, carbon-germanium, and silicon-germanium triangulenes. *Journal of Computational Chemistry*, 36(29):2193–2199, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guo:2019:MRO

[GSMZ19] Shuaifei Guo, Cuihong Sun, Lingpeng Meng, and Yanli Zeng. The mechanism of ring-opening polymerization of L-lactide by ICl_3 catalysts: Halogen bond catalysis or participating in reactions? *Journal of Computational Chemistry*, 40(32): 2827–2833, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gotz:2013:PDF

[GSS13] Daniel A. Götz, Rolf Schäfer, and Peter Schwerdtfeger. The performance of density functional and wavefunction-based methods for 2D and 3D structures of Au_{10}. *Journal of Computational Chemistry*, 34(23):1975–1981, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gogtas:2010:TDQ

[GTK10] Fahrettin Gogtas, Rukiye Tutuk, and Mustafa Kurban. Time-dependent quantum study of $H(^2S)$ + $FO(^2\Pi\ )$ $\rightarrow$ $OH(^2\Pi\ )$ + $F(^2P)$ reaction on the 1^3A' and 1^3A" states. *Journal of Computational Chemistry*, 31(14):2607–2611, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garbounis:2010:SEB

[GTT10] Dimitrios N. Garbounis, Athanassios C. Tsipis, and Constantinos A. Tsipis. Structural, electronic, bonding, magnetic, and optical properties of bimetallic $[Ru_nAu_m\ ]^{0/+}$ $(n + m \leq 3$) clusters. *Journal of Computational Chemistry*, 31(16):2836–2852, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guruge:2018:BFP

[GTZ+18] Ivantha Guruge, Ghazaleh Taherzadeh, Jian Zhan, Yaoqi Zhou, and Yuedong Yang. B-factor profile prediction for RNA flexibility using support vector machines. *Journal of Computational Chemistry*, 39(8):407–411, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghysels:2010:CSV

[GVP+10] An Ghysels, Veronique Van Speybroeck, Ewald Pauwels, Saron Catak, Bernard R. Brooks, Dimitri Van Neck, and

Michel Waroquier. Comparative study of various normal mode analysis techniques based on partial Hessians. *Journal of Computational Chemistry*, 31(5):994–1007, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ganesan:2011:IIP

[GWF11] Aravindhan Ganesan, Feng Wang, and Chantal Falzon. Intramolecular interactions of L-phenylalanine: Valence ionization spectra and orbital momentum distributions of its fragment molecules. *Journal of Computational Chemistry*, 32(3): 525–535, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gutsev:2012:SPA

[GWJJ12] Gennady L. Gutsev, Charles A. Weatherford, Lewis E. Johnson, and Purusottam Jena. Structure and properties of the aluminum borates $Al(BO_2)_n$ and $Al(BO_2)_n^-$, (n = 1–4). *Journal of Computational Chemistry*, 33(4):416–424, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goel:2018:PDF

[GWJR18] Himanshu Goel, Zachary W. Windom, Amber A. Jackson, and Neeraj Rai. Performance of density functionals for modeling vapor liquid equilibria of CO_2 and SO_2. *Journal of Computational Chemistry*, 39(8):397–406, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gutsev:2011:DFS

[GWPJ11] G. L. Gutsev, C. A. Weatherford, K. Pradhan, and P. Jena. Density functional study of neutral and anionic AlO_n and ScO_n with high oxygen content. *Journal of Computational Chemistry*, 32(14):2974–2982, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gan:2017:CCB

[GWT+17] Li-Hua Gan, Rui Wu, Jian-Lei Tian, Joseph Clarke, Christopher Gibson, and Patrick W. Fowler. From C_{58} to C_{62} and back: Stability, structural similarity, and ring current. *Journal of Computational Chemistry*, 38(3):144–151, January 30,

2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Glendening:2019:EON

[GWW19] Eric D. Glendening, Stephen J. Wright, and Frank Weinhold. Efficient optimization of natural resonance theory weightings and bond orders by gram-based convex programming. *Journal of Computational Chemistry*, 40(23):2028–2035, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gu:2012:SEP

[GWX+12] Jiande Gu, Jing Wang, Yaoming Xie, Jerzy Leszczynski, and Henry F. Schaefer III. Structural and electronic property responses to the arsenic/phosphorus exchange in GC-related DNA of the *B*-form. *Journal of Computational Chemistry*, 33(8):817–821, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gong:2015:TVH

[GWZ15] Wenjing Gong, Ruibo Wu, and Yingkai Zhang. Thiol versus hydroxamate as zinc binding group in HDAC inhibition: An ab initio QM/MM molecular dynamics study. *Journal of Computational Chemistry*, 36(30):2228–2235, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guo:2012:XEO

[GWZX12] Wenping Guo, Anan Wu, Igor Ying Zhang, and Xin Xu. XO: an extended ONIOM method for accurate and efficient modeling of large systems. *Journal of Computational Chemistry*, 33 (27):2142–2160, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gong:2010:IMS

[GY10] Li-Dong Gong and Zhong-Zhi Yang. Investigation of the molecular surface area and volume: Defined and calculated by the molecular face theory. *Journal of Computational Chemistry*, 31(11):2098–2108, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guan:2012:KHA

[GY12] Yulei Guan and Bolun Yang. Kinetics for the hydrogen-abstraction of CH_4 with NO_2. *Journal of Computational Chemistry*, 33(23):1870–1879, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2010:TSG

[GYX+10] Chao Gao, Hua-Qing Yang, Jian Xu, Song Qin, and Chang-Wei Hu. Theoretical study on the gas-phase reaction mechanism between rhodium monoxide and methane for methanol production. *Journal of Computational Chemistry*, 31(5):938–953, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grinter:2014:BSA

[GZ14] Sam Z. Grinter and Xiaoqin Zou. A Bayesian statistical approach of improving knowledge-based scoring functions for protein–ligand interactions. *Journal of Computational Chemistry*, 35(12):932–943, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gan:2010:NFH

[GZH10] Li-Hua Gan, Jian-Qiang Zhao, and Qun Hui. Nonclassical fullerenes with a heptagon violating the pentagon adjacency penalty rule. *Journal of Computational Chemistry*, 31(8):1715–1721, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2012:MRN

[GZL+12] Jie Ying Gao, Cheng Hua Zhang, Mei Ming Luo, Chan Kyung Kim, Wei Chu, and Ying Xue. Mechanism for the reaction of 2-naphthol with N-methyl-N-phenyl-hydrazine suggested by the density functional theory investigations. *Journal of Computational Chemistry*, 33(2):220–230, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grosdidier:2011:FDU

[GZM11] Aurélien Grosdidier, Vincent Zoete, and Olivier Michielin. Fast docking using the CHARMM force field with EADock DSS. *Journal of Computational Chemistry*, 32(10):2149–2159, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guo:2012:ICS

[GZZ12] Xu-Geng Guo, Jing-Lai Zhang, and Yuan Zhao. Ab initio characterization of size dependence of electronic spectra for linear anionic carbon clusters C_n^- ($n = 4$–17). *Journal of Computational Chemistry*, 33(1):93–102, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2016:CSG

[GZZM16] Lei Gao, Yanli Zeng, Xueying Zhang, and Lingpeng Meng. Comparative studies on group III σ-hole and π-hole interactions. *Journal of Computational Chemistry*, 37(14):1321–1327, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hahn:2010:IRE

[HAGK10] Seungsoo Hahn, Orr Ashenberg, Gevorg Grigoryan, and Amy E. Keating. Identifying and reducing error in cluster-expansion approximations of protein energies. *Journal of Computational Chemistry*, 31(16):2900–2914, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holmes:2016:ABV

[HAI+16] Sean T. Holmes, Fahri Alkan, Robbie J. Iuliucci, Karl T. Mueller, and Cecil Dybowski. Analysis of the bond-valence method for calculating ^{29}Si and ^{31}P magnetic shielding in covalent network solids. *Journal of Computational Chemistry*, 37(18):1704–1710, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heinen:2014:HAE

[HAL14] Marco Heinen, Elshad Allahyarov, and Hartmut Löwen. Highly asymmetric electrolytes in the primitive model: Hypernetted chain solution in arbitrary spatial dimensions. *Journal of Computational Chemistry*, 35(4):275–289, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hamacher:2011:EQI

[Ham11] Kay Hamacher. Efficient quantification of the importance of contacts for the dynamical stability of proteins. *Journal of Computational Chemistry*, 32(5):810–815, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hanke:2011:SAU

[Han11] Felix Hanke. Sensitivity analysis and uncertainty calculation for dispersion corrected density functional theory. *Journal of Computational Chemistry*, 32(7):1424–1430, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hofinger:2012:GAC

[HAP+12] Siegfried Höfinger, Angela Acocella, Sergiu C. Pop, Tetsu Narumi, Kenji Yasuoka, Titus Beu, and Francesco Zerbetto. GPU-accelerated computation of electron transfer. *Journal of Computational Chemistry*, 33(29):2351–2356, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hassan:2014:ITS

[Has14] Sergio A. Hassan. Implicit treatment of solvent dispersion forces in protein simulations. *Journal of Computational Chemistry*, 35(22):1621–1629, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hacene:2012:AVE

[HASR+12] Mohamed Hacene, Ani Anciaux-Sedrakian, Xavier Rozanska, Diego Klahr, Thomas Guignon, and Paul Fleurat-Lessard. Accelerating VASP electronic structure calculations using graphic processing units. *Journal of Computational Chemistry*, 33(32):2581–2589, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heit:2014:ESG

[HB14] Yonaton Heit and Gregory J. O. Beran. Exploiting space-group symmetry in fragment-based molecular crystal calculations. *Journal of Computational Chemistry*, 35(30):2205–2214, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hochheim:2015:AIC

[HB15] Manuel Hochheim and Thomas Bredow. Adsorption-induced changes of intramolecular optical transitions: PTCDA/NaCl and PTCDA/KCl. *Journal of Computational Chemistry*, 36 (24):1805–1811, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hohnerbach:2019:AAN

[HB19] Markus Höhnerbach and Paolo Bientinesi. Accelerating AIREBO: Navigating the journey from legacy to high-performance code. *Journal of Computational Chemistry*, 40 (14):1471–1482, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holmes:2017:CSS

[HBI+17] Sean T. Holmes, Shi Bai, Robbie J. Iuliucci, Karl T. Mueller, and Cecil Dybowski. Calculations of solid-state ^{43}Ca NMR parameters: a comparison of periodic and cluster approaches and an evaluation of DFT functionals. *Journal of Computational Chemistry*, 38(13):949–956, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hsu:2017:SNU

[HBJ+17] Pin-Chia Hsu, Bart M. H. Bruininks, Damien Jefferies, Paulo Cesar Telles de Souza, Jumin Lee, Dhilon S. Patel, Siewert J. Marrink, Yifei Qi, Syma Khalid, and Wonpil Im. Software news and updates: CHARMM-GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. *Journal of Computational Chemistry*, 38 (27):2354–2363, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holt:2010:NPI

[HBKL10] Asbjørn Holt, Jonas Boström, Gunnar Karlström, and Roland Lindh. A NEMO potential that includes the dipole–quadrupole and quadrupole–quadrupole polarizability. *Journal of Computational Chemistry*, 31(8):1583–1591, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Honigmann:2012:CCI

[HBL12] Michael Honigmann, Robert J. Buenker, and Heinz-Peter Liebermann. Complex configuration interaction calculations of the cross section for the dissociative electron attachment process e^{-} + F_2 → F → F + F^{-} using the complex basis function method. *Journal of Computational Chemistry*, 33(4):355–362, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hurd:2017:QMS

[HBR17] Catherine A. Hurd, Nicholas A. Besley, and David Robinson. A QM/MM study of the nature of the entatic state in plastocyanin. *Journal of Computational Chemistry*, 38(16):1431–1437, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hynninen:2014:SNU

[HC14] Antti-Pekka Hynninen and Michael F. Crowley. Software news and updates: New faster CHARMM molecular dynamics engine. *Journal of Computational Chemistry*, 35(5):406–413, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Halbert:2011:SGB

[HCB11] Stéphanie Halbert, Carine Clavaguéra, and Guy Bouchoux. The shape of gaseous n-butylbenzene: Assessment of computational methods and comparison with experiments. *Journal of Computational Chemistry*, 32(8):1550–1560, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hendrickx:2010:UTA

[HCD+10] Pieter M. S. Hendrickx, Francisco Corzana, Stefaan Depraetere, Dirk A. Tourwé, Koen Augustyns, and José C. Martins. The use of time-averaged $^{3}J_{HH}$ restrained molecular dynamics (tar-MD) simulations for the conformational analysis of five-membered ring systems: Methodology and applications. *Journal of Computational Chemistry*, 31(3):561–572, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hughes:2015:RSA

[HCP15] Timothy J. Hughes, Salvatore Cardamone, and Paul L. A. Popelier. Realistic sampling of amino acid geometries for a multipolar polarizable force field. *Journal of Computational Chemistry*, 36(24):1844–1857, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heinz:2015:TSI

[HDB15] Norah Heinz, Michael Dolg, and Albrecht Berkessel. A theoretical study of imine hydrocyanation catalyzed by halogen-bonding. *Journal of Computational Chemistry*, 36(24):1812–1817, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hellweg:2012:SNU

[HDH12] Arnim Hellweg, Michael Diedenhofen, and Uwe Huniar. Software news and updates: `thermocalc` — a poor man's approach to computational thermochemistry. *Journal of Computational Chemistry*, 33(8):881–886, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2015:ETAa

[HDHL15a] Jing Huang, Likai Du, Deping Hu, and Zhenggang Lan. Erratum: Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. *Journal of Computational Chemistry*, 36(24):1858, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HDHL15c].

Huang:2015:ETAb

[HDHL15b] Jing Huang, Likai Du, Deping Hu, and Zhenggang Lan. Erratum: Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. *Journal of Computational Chemistry*, 36(29):2208, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HDHL15a].

Huang:2015:TAE

[HDHL15c] Jing Huang, Likai Du, Deping Hu, and Zhenggang Lan. Theoretical analysis of excited states and energy transfer mechanism in conjugated dendrimers. *Journal of Computational*

Chemistry, 36(3):151–163, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [HDHL15a, HDHL15b].

Hansen:2012:AED

[HDK+12] Niels Hansen, Jožica Dolenc, Matthias Knecht, Sereina Riniker, and Wilfred F. van Gunsteren. Assessment of enveloping distribution sampling to calculate relative free enthalpies of binding for eight netropsin–DNA duplex complexes in aqueous solution. *Journal of Computational Chemistry*, 33 (6):640–651, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hildebrandt:2014:ECR

[HDL+14] Anna K. Hildebrandt, Matthias Dietzen, Thomas Lengauer, Hans-Peter Lenhof, Ernst Althaus, and Andreas Hildebrandt. Efficient computation of root mean square deviations under rigid transformations. *Journal of Computational Chemistry*, 35(10):765–771, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harris:2017:CCF

[HDL+17] Robert C. Harris, Nanjie Deng, Ronald M. Levy, Ryosuke Ishizuka, and Nobuyuki Matubayasi. Computing conformational free energy differences in explicit solvent: an efficient thermodynamic cycle using an auxiliary potential and a free energy functional constructed from the end points. *Journal of Computational Chemistry*, 38(15):1198–1208, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higo:2015:VSC

[HDM+15] Junichi Higo, Bhaskar Dasgupta, Tadaaki Mashimo, Kota Kasahara, Yoshifumi Fukunishi, and Haruki Nakamura. Virtual-system-coupled adaptive umbrella sampling to compute free-energy landscape for flexible molecular docking. *Journal of Computational Chemistry*, 36(20):1489–1501, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hattab:2019:SBE

[HDM+19] Awatef Hattab, Zoubeida Dhaouadi, Alhadji Malloum, Jean Jules Fifen, Souad Lahmar, Nino Russo, and Emilia

Sicilia. Structures, binding energies, temperature effects, infrared spectroscopy of $[Mg(NH_3)_{n=1--10}]^+$ clusters from DFT and MP2 investigations. *Journal of Computational Chemistry*, 40(18):1707–1717, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hofmann:2014:TFF

[HDPM14] Franziska D. Hofmann, Michael Devereux, Andreas Pfaltz, and Markus Meuwly. Toward force fields for atomistic simulations of iridium-containing complexes. *Journal of Computational Chemistry*, 35(1):18–29, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heinz:2010:CSB

[Hei10] Hendrik Heinz. Computational screening of biomolecular adsorption and self-assembly on nanoscale surfaces. *Journal of Computational Chemistry*, 31(7):1564–1568, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heinen:2018:CPP

[Hei18] Marco Heinen. Calculating particle pair potentials from fluid-state pair correlations: Iterative Ornstein–Zernike inversion. *Journal of Computational Chemistry*, 39(20):1531–1543, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hellweg:2013:HCK

[Hel13] Arnim Hellweg. Heuristic control of kinetic energy in dynamic reaction coordinate calculations. *Journal of Computational Chemistry*, 34(21):1835–1841, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huhn:2017:IES

[HEM+17] Carolin Hühn, Andreas Erlebach, Dorothea Mey, Lothar Wondraczek, and Marek Sierka. Ab Initio energetics of SiO bond cleavage. *Journal of Computational Chemistry*, 38(27):2349–2353, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hernandez-Esparza:2014:GBA

[HEMCZE+14] Raymundo Hernández-Esparza, Sol-Milena Mejía-Chica, Andy D. Zapata-Escobar, Alfredo Guevara-García, Apolinar

Martínez-Melchor, Julio-M. Hernández-Pérez, Rubicelia Vargas, and Jorge Garza. Grid-based algorithm to search critical points, in the electron density, accelerated by graphics processing units. *Journal of Computational Chemistry*, 35(31): 2272–2278, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hess:2019:EIC

[Hes19] Franziska Hess. Efficient implementation of cluster expansion models in surface kinetic Monte Carlo simulations with lateral interactions: Subtraction schemes, supersites, and the supercluster contraction. *Journal of Computational Chemistry*, 40(30):2664–2676, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hess:2012:FPK

[HFSO12] Franziska Hess, Attila Farkas, Ari P. Seitsonen, and Herbert Over. "first-principles" kinetic Monte Carlo simulations revisited: CO oxidation over $RuO_2(110)$. *Journal of Computational Chemistry*, 33(7):757–766, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holland:2010:EEC

[HG10] Jason P. Holland and Jennifer C. Green. Evaluation of exchange-correlation functionals for time-dependent density functional theory calculations on metal complexes. *Journal of Computational Chemistry*, 31(5):1008–1014, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Homeyer:2013:SNU

[HG13] Nadine Homeyer and Holger Gohlke. Software news and updates: FEW: a workflow tool for free energy calculations of ligand binding. *Journal of Computational Chemistry*, 34(11): 965–973, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holguin-Gallego:2016:ECI

[HGCCGR+16] Fernando José Holguín-Gallego, Rodrigo Chávez-Calvillo, Marco García-Revilla, Evelio Francisco, Ángel Martín Pendás, and Tomás Rocha-Rinza. Electron correlation in the interacting quantum atoms partition via coupled-cluster Lagrangian densities. *Journal of Computational Chemistry*, 37(19):1753–1765, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoffmann:2014:IID

[HGHP14] Alexander Hoffmann, Richard Grunzke, and Sonja Herres-Pawlis. Insights into the influence of dispersion correction in the theoretical treatment of guanidine–quinoline copper(I) complexes. *Journal of Computational Chemistry*, 35(27):1943–1950, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2018:WLS

[HGW18] Dan Hu, Xiaoqing Guan, and Yukun Wang. Weighted least square analysis method for free energy calculations. *Journal of Computational Chemistry*, 39(28):2397–2404, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2015:NAR

[HGY15] Ming Huang, Timothy J. Giese, and Darrin M. York. Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. *Journal of Computational Chemistry*, 36(18):1370–1389, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hansen:2010:ULE

[HH10] Halvor S. Hansen and Philippe H. Hünenberger. Using the local elevation method to construct optimized umbrella sampling potentials: Calculation of the relative free energies and interconversion barriers of glucopyranose ring conformers in water. *Journal of Computational Chemistry*, 31(1):1–23, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hansen:2011:RGF

[HH11] Halvor S. Hansen and Philippe H. Hünenberger. A reoptimized GROMOS force field for hexopyranose-based carbohydrates accounting for the relative free energies of ring conformers, anomers, epimers, hydroxymethyl rotamers, and glycosidic linkage conformers. *Journal of Computational Chemistry*, 32(6):998–1032, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hitzenberger:2015:PRA

[HH15] Manuel Hitzenberger and Thomas S. Hofer. Probing the range of applicability of structure- and energy-adjusted QM/MM link bonds. *Journal of Computational Chemistry*, 36(26): 1929–1939, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heuser:2016:WFF

[HH16a] Johannes Heuser and Sebastian Höfener. Wave-function frozen-density embedding: Approximate analytical nuclear ground-state gradients. *Journal of Computational Chemistry*, 37(12):1092–1101, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Holec:2016:SNU

[HH16b] Patrick V. Holec and Benjamin J. Hackel. Software news and updates: PyMOL360: Multi-user gamepad control of molecular visualization software. *Journal of Computational Chemistry*, 37(30):2667–2669, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heuser:2017:ANE

[HH17] Johannes Heuser and Sebastian Höfener. Analytical nuclear excited-state gradients for the Tamm–Dancoff approximation using uncoupled frozen-density embedding. *Journal of Computational Chemistry*, 38(27):2316–2325, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higham:2018:OLC

[HH18] Jonathan Higham and Richard H. Henchman. Overcoming the limitations of cutoffs for defining atomic coordination in multicomponent systems. *Journal of Computational Chemistry*, 39(12):705–710, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2010:GDM

[HHBY10] Xiangqian Hu, Hao Hu, David N. Beratan, and Weitao Yang. A gradient-directed Monte Carlo approach for protein design. *Journal of Computational Chemistry*, 31(11):2164–2168, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Herrmann:2016:QCS

[HHDC16] Nils Herrmann, Norah Heinz, Michael Dolg, and Xiaoyan Cao. Quantum chemical study of the autoxidation of ascorbate. *Journal of Computational Chemistry*, 37(20):1914–1923, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayami:2019:MVS

[HHNK19] Tomonori Hayami, Junichi Higo, Haruki Nakamura, and Kota Kasahara. Multidimensional virtual-system coupled canonical molecular dynamics to compute free-energy landscapes of peptide multimer assembly. *Journal of Computational Chemistry*, 40(28):2453–2463, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hischenhuber:2013:CDG

[HHT+13a] B. Hischenhuber, H. Havlicek, J. Todoric, S. Höllrigl-Binder, W. Schreiner, and B. Knapp. Corrigendum: Differential geometric analysis of alterations in MHα-helices. *Journal of Computational Chemistry*, 34(32):2834, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HHT+13b].

Hischenhuber:2013:SNU

[HHT+13b] Birgit Hischenhuber, Hans Havlicek, Jelena Todoric, Sonja Höllrigl-Binder, Wolfgang Schreiner, and Bernhard Knapp. Software news and updates: Differential geometric analysis of alterations in MHα-helices. *Journal of Computational Chemistry*, 34(21):1862–1879, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See corrigendum [HHT+13a].

Huang:2017:EEB

[HHWL17] Ming Huang, Wenjun Huang, Fei Wen, and Ronald G. Larson. Efficient estimation of binding free energies between peptides and an MHC class II molecule using coarse-grained molecular dynamics simulations with a weighted histogram analysis method. *Journal of Computational Chemistry*, 38(23):2007–2019, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hill:2013:ABS

[Hil13] J. Grant Hill. Auxiliary basis sets for density-fitting second-order Møller–Plesset perturbation theory: Weighted core-valence correlation consistent basis sets for the $4d$ elements Y–Pd. *Journal of Computational Chemistry*, 34(25):2168–2177, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirst:2017:ISB

[HIS17] Jonathan Hirst, Wonpil Im, and Joan-Emma Shea. Introduction: Simulating biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. *Journal of Computational Chemistry*, 38(15):1111–1113, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2010:ABF

[HJ10] Zhongqiao Hu and Jianwen Jiang. Assessment of biomolecular force fields for molecular dynamics simulations in a protein crystal. *Journal of Computational Chemistry*, 31(2):371–380, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hnyk:2013:CCC

[HJ13] Drahomír Hnyk and Elambalassery G. Jayasree. Cationic Closo-carboranes 2. Do computed ^{11}B and ^{13}C NMR chemical shifts support their experimental availability? *Journal of Computational Chemistry*, 34(8):656–661, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heine:2009:CCW

[HJG09] Thomas Heine, Jan-Ole Joswig, and Achim Gelessus. *Computational Chemistry Workbook: Learning Through Examples*. Wiley-VCH, Weinheim, Germany, 2009. ISBN 3-527-32442-9. xvii + 232 pp. LCCN QD39.3.M3 H45 2009. URL http://www.loc.gov/catdir/enhancements/fy1009/2010279275-b.html; http://www.loc.gov/catdir/enhancements/fy1009/2010279275-d.html; http://www.loc.gov/catdir/enhancements/fy1009/2010279275-t.html. With a foreword by Dennis R. Salahub.

Hoyvik:2013:PML

[HJJ13] Ida-Marie Høyvik, Branislav Jansik, and Poul Jørgensen. Pipek–Mezey localization of occupied and virtual orbitals. *Journal of Computational Chemistry*, 34(17):1456–1462, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoyvik:2013:LHF

[HJKJ13] Ida-Marie Høyvik, Branislav Jansik, Kasper Kristensen, and Poul Jørgensen. Local Hartree–Fock orbitals using a three-level optimization strategy for the energy. *Journal of Computational Chemistry*, 34(15):1311–1320, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hubin:2016:PRR

[HJLV16] Pierre O. Hubin, Denis Jacquemin, Laurence Leherte, and Daniel P. Vercauteren. Parameterization of the ReaxFF reactive force field for a proline-catalyzed aldol reaction. *Journal of Computational Chemistry*, 37(29):2564–2572, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hamilton:2018:PGR

[HK18] John Hamilton and Evangelia Kotsikorou. Parameterization of the GPR119 receptor agonist AR231453. *Journal of Computational Chemistry*, 39(1):35–41, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayami:2018:MDC

[HKNH18] Tomonori Hayami, Kota Kasahara, Haruki Nakamura, and Junichi Higo. Molecular dynamics coupled with a virtual system for effective conformational sampling. *Journal of Computational Chemistry*, 39(19):1291–1299, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heinzerling:2012:FFF

[HKR12] Lennart Heinzerling, Robert Klein, and Matthias Rarey. Fast force field-based optimization of protein–ligand complexes with graphics processor. *Journal of Computational Chemistry*, 33(32):2554–2565, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hrda:2014:SNU

[HKR+14] Marcela Hrdá, Tomáš Kulich, Michal Repiský, Jozef Noga, Olga L. Malkina, and Vladimir G. Malkin. Software news and updates: Implementation of the diagonalization-free algorithm in the self-consistent field procedure within the four-component relativistic scheme. *Journal of Computational Chemistry*, 35(23):1725–1737, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hahnke:2011:PASa

[HKRS11] Volker Hähnke, Alexander Klenner, Friedrich Rippmann, and Gisbert Schneider. Pharmacophore alignment search tool: Influence of the third dimension on text-based similarity searching. *Journal of Computational Chemistry*, 32(8):1618–1634, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2014:SNU

[HL14] Bingjie Hu and Markus A. Lill. Software news and updates: WATsite: Hydration site prediction program with PyMOL interface. *Journal of Computational Chemistry*, 35(16):1255–1260, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2019:ITD

[HL19] Chao Huang and Wenjian Liu. iVI-TD-DFT: an iterative vector interaction method for exterior/interior roots of TD-DFT. *Journal of Computational Chemistry*, 40(9):1023–1037, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hintze:2015:SSS

[HLB15] Kim Julia Hintze, Arne Lützen, and Thomas Bredow. Structure and stability of supramolecular crown ether complexes. *Journal of Computational Chemistry*, 36(19):1467–1472, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hernandez-Lima:2015:RIC

[HLBLCCG15] Joseelyne G. Hernández-Lima, Jose E. Barquera-Lozada, Gabriel Cuevas, and Fernando Cortés-Guzmán. The role of induced current density in stereoelectronic effects: Perlin effect. *Journal of Computational Chemistry*, 36(21):1573–1578, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2018:MDS

[HLEM18] Jing Huang, Justin A. Lemkul, Peter K. Eastman, and Alexander D. MacKerell Jr. Molecular dynamics simulations using the drude polarizable force field on GPUs with OpenMM: Implementation, validation, and benchmarks. *Journal of Computational Chemistry*, 39(21):1682–1689, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Horta:2012:RIP

[HLH+12] Bruno A. C. Horta, Zhixiong Lin, Wei Huang, Sereina Riniker, Wilfred F. van Gunsteren, and Philippe H. Hünenberger. Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: Influence on the folding properties of two beta-peptides in methanol. *Journal of Computational Chemistry*, 33(24): 1907–1917, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayashi:2019:HIM

[HLI+19] Taku Hayashi, Ka Hung Lee, Hiroki Iida, Eiji Yashima, Stephan Irle, and Yuh Hijikata. The helix-inversion mechanism in double-stranded helical oligomers bridged by rotary cyclic boronate esters. *Journal of Computational Chemistry*, 40(23):2036–2042, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Han:2012:CMB

[HLS12] Yunqing Han, Tianxiang Li, and Kozo Saito. Comprehensive method based on model free method and IKP method for evaluating kinetic parameters of solid state reactions. *Journal of Computational Chemistry*, 33(31):2516–2525, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

He:2013:SNU

[HLS+13] Yuye He, Chin Yee Liew, Nitin Sharma, Sze Kwang Woo, Yi Ting Chau, and Chun Wei Yap. Software news and updates: PaDEL-DDPredictor: Open-source software for PD-PK-T prediction. *Journal of Computational Chemistry*, 34 (7):604–610, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Herbers:2013:RGC

[HLvdV13] Claudia R. Herbers, Chunli Li, and Nico F. A. van der Vegt. Reviews: Grand challenges in quantum-classical modeling of molecule–surface interactions. *Journal of Computational Chemistry*, 34(14):1177–1188, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harger:2017:TOA

[HLW+17] Matthew Harger, Daniel Li, Zhi Wang, Kevin Dalby, Louis Lagardère, Jean-Philip Piquemal, Jay Ponder, and Pengyu Ren. Tinker–OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. *Journal of Computational Chemistry*, 38(23):2047–2055, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2015:ESM

[HLWD15] Jin-Dou Huang, Wen-Liang Li, Shu-Hao Wen, and Bin Dong. Electronic structure and microscopic charge-transport properties of a new-type diketopyrrolopyrrole-based material. *Journal of Computational Chemistry*, 36(10):695–706, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2017:IIV

[HLXH17] Chao Huang, Wenjian Liu, Yunlong Xiao, and Mark R. Hoffmann. iVI: an iterative vector interaction method for large eigenvalue problems. *Journal of Computational Chemistry*, 38(29):2481–2499, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [HLXH18].

Huang:2018:EII

[HLXH18] Chao Huang, Wenjian Liu, Yunlong Xiao, and Mark R. Hoffmann. Erratum: “iVI: an iterative vector interaction method for large eigenvalue problems” [J. Comput. Chem. **38**, 2481 (2017)]. *Journal of Computational Chemistry*, 39(6):338, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HLXH17].

Huang:2013:CAA

[HM13] Jing Huang and Alexander D. MacKerell Jr. CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data. *Journal of Computational Chemistry*, 34(25):2135–2145, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hills:2016:MPS

[HM16] Ronald D. Hills Jr. and Nicholas McGlinchey. Model parameters for simulation of physiological lipids. *Journal of Computational Chemistry*, 37(12):1112–1118, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hongo:2010:RNG

[HMM10] Kenta Hongo, Ryo Maezono, and Kenichi Miura. Random number generators tested on quantum Monte Carlo simulations. *Journal of Computational Chemistry*, 31(11):2186–2194, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hallen:2018:OOS

[HMO+18] Mark A. Hallen, Jeffrey W. Martin, Adegoke Ojewole, Jonathan D. Jou, Anna U. Lowegard, Marcel S. Frenkel, Pablo Gainza, Hunter M. Nisonoff, Aditya Mukund, Siyu Wang, Graham T. Holt, David Zhou, Elizabeth Dowd, and Bruce R. Donald. OSPREY 3.0: Open-source protein redesign for you, with powerful new features. *Journal of Computational Chemistry*, 39(30):2494–2507, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hall:2013:EPS

[HNHR13] Vincent Hall, Anthony Nash, Evor Hines, and Alison Rodger. Elucidating protein secondary structure with circular dichroism and a neural network. *Journal of Computational Chemistry*, 34(32):2774–2786, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirano:2017:PAC

[HNN+17] Kenji Hirano, Hiroshi Nakano, Yoshihide Nakao, Hirofumi Sato, and Shigeyoshi Sakaki. Photo absorption of *p*-coumaric acid in aqueous solution: RISM–SCF–SEDD theory approach. *Journal of Computational Chemistry*, 38(18):1567–1573, July

5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2016:SWO

[HNS16] Ryuhei Harada, Tomotake Nakamura, and Yasuteru Shigeta. Sparsity-weighted outlier FLOODing (OFLOOD) method: Efficient rare event sampling method using sparsity of distribution. *Journal of Computational Chemistry*, 37(8):724–738, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2015:PFP

[HNTS15] Ryuhei Harada, Tomotake Nakamura, Yu Takano, and Yasuteru Shigeta. Protein folding pathways extracted by OFLOOD: Outlier FLOODing method. *Journal of Computational Chemistry*, 36(2):97–102, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heringer:2007:AES

[HNWF07] D. Heringer, T. A. Niehaus, M. Wanko, and Th. Frauenheim. Analytical excited state forces for the time-dependent density-functional tight-binding method. *Journal of Computational Chemistry*, 28(16):2589–2601, December 2007. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [HNWF12].

Heringer:2012:EAE

[HNWF12] D. Heringer, T. A. Niehaus, M. Wanko, and Th. Frauenheim. Erratum: "Analytical excited state forces for the time-dependent density-functional tight-binding method" [J. Comp. Chem. **28**, 2589]. *Journal of Computational Chemistry*, 33(5):593, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HNWF07].

Harada:2019:CSO

[HNyH19] Iori Harada, Akira Nakayama, and Jun ya Hasegawa. Constraint structure optimization to a specific minimum using ionization energy. *Journal of Computational Chemistry*, 40 (2):507–514, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hofener:2014:CCF

[Höf14] Sebastian Höfener. Coupled-cluster frozen-density embedding using resolution of the identity methods. *Journal of Computational Chemistry*, 35(23):1716–1724, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hrsak:2017:OTN

[HOK17] Dalibor Hršak, Jógvan Magnus Haugaard Olsen, and Jacob Kongsted. Optimization and transferability of non-electrostatic repulsion in the polarizable density embedding model. *Journal of Computational Chemistry*, 38(24):2108–2117, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harabuchi:2016:NST

[HOM+16] Yu Harabuchi, Yuriko Ono, Satoshi Maeda, Tetsuya Taketsugu, Kristopher Keipert, and Mark S. Gordon. Nontotally symmetric trifurcation of an S_N2 reaction pathway. *Journal of Computational Chemistry*, 37(5):487–493, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haque:2010:PAP

[HP10a] Imran S. Haque and Vijay S. Pande. PAPER — accelerating parallel evaluations of ROCS. *Journal of Computational Chemistry*, 31(1):117–132, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Henriksson:2010:PDT

[HP10b] Krister O. E. Henriksson and Janne Pesonen. Polymer dynamics in torsion space. *Journal of Computational Chemistry*, 31 (9):1882–1888, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

He:2013:MPB

[HPL13] Yi He, Lidia Prieto, and Themis Lazaridis. Modeling peptide binding to anionic membrane pores. *Journal of Computational Chemistry*, 34(17):1463–1475, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heffernan:2018:SSB

[HPL+18] Rhys Heffernan, Kuldip Paliwal, James Lyons, Jaswinder Singh, Yuedong Yang, and Yaoqi Zhou. Single-sequence-based prediction of protein secondary structures and solvent accessibility by deep whole-sequence learning. *Journal of Computational Chemistry*, 39(26):2210–2216, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hinsen:2012:SNU

[HPSK12] Konrad Hinsen, Eric Pellegrini, Sławomir Stachura, and Gerald R. Kneller. Software news and updates: n Moldyn 3: Using task farming for a parallel spectroscopy-oriented analysis of molecular dynamics simulations. *Journal of Computational Chemistry*, 33(25):2043–2048, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heggen:2016:CUH

[HPT16a] Berit Heggen, Mahendra Patil, and Walter Thiel. Cyclization of an α, β-unsaturated hydrazone catalyzed by a BINOL-phosphoric acid: Pericyclic or not? *Journal of Computational Chemistry*, 37(2):280–285, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hermann:2016:SNU

[HPT+16b] Gunter Hermann, Vincent Pohl, Jean Christophe Tremblay, Beate Paulus, Hans-Christian Hege, and Axel Schild. Software news and updates: ORBKIT: a modular Python toolbox for cross-platform postprocessing of quantum chemical wavefunction data. *Journal of Computational Chemistry*, 37(16): 1511–1520, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hermann:2017:OSF

[HPT17] Gunter Hermann, Vincent Pohl, and Jean Christophe Tremblay. An open-source framework for analyzing N-electron dynamics. II. Hybrid density functional theory/configuration interaction methodology. *Journal of Computational Chemistry*, 38(28):2378–2387, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Howell:2016:MCS

[HQC16] Steven C. Howell, Xiangyun Qiu, and Joseph E. Curtis. Monte Carlo simulation algorithm for B-DNA. *Journal of Computational Chemistry*, 37(29):2553–2563, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2019:CHS

[HQSZ19] Dading Huang, Yifei Qi, Jianing Song, and John Z. H. Zhang. Calculation of hot spots for protein-protein interaction in p53/PMI-MDM2/ MDMX complexes. *Journal of Computational Chemistry*, 40(9):1045–1056, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heimbach:2017:SNU

[HRB+17] Ingo Heimbach, Florian Rhiem, Fabian Beule, David Knodt, Josef Heinen, and Robert O. Jones. Software news and updates: pyMolDyn: Identification, structure, and properties of cavities/vacancies in condensed matter and molecules. *Journal of Computational Chemistry*, 38(6):389–394, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harano:2013:MAA

[HRC13] Yuichi Harano, Roland Roth, and Shuntaro Chiba. A morphometric approach for the accurate solvation thermodynamics of proteins and ligands. *Journal of Computational Chemistry*, 34 (23):1969–1974, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Husseini:2017:CIS

[HRH+17] Fouad S. Husseini, David Robinson, Neil T. Hunt, Anthony W. Parker, and Jonathan D. Hirst. Computing infrared spectra of proteins using the exciton model. *Journal of Computational Chemistry*, 38(16):1362–1375, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2017:EBE

[HRHI17] Qi Huang, Jocelyn M. Rodgers, Russell J. Hemley, and Toshiko Ichiye. Extreme biophysics: Enzymes under pressure. *Journal of Computational Chemistry*, 38(15):1174–1182, June

5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huwald:2016:CMD

[HRID16] Jan Huwald, Stephan Richter, Bashar Ibrahim, and Peter Dittrich. Compressing molecular dynamics trajectories: Breaking the one-bit-per-sample barrier. *Journal of Computational Chemistry*, 37(20):1897–1906, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoffmann:2014:GOB

[HRJ+14] Alexander Hoffmann, Martin Rohrmüller, Anton Jesser, Ines dos Santos Vieira, Wolf Gero Schmidt, and Sonja Herres-Pawlis. Geometrical and optical benchmarking of copper(II) guanidine–quinoline complexes: Insights from TD–DFT and many-body perturbation theory (part II). *Journal of Computational Chemistry*, 35(29):2146–2161, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See corrigendum [HRJ+15].

Hoffmann:2015:ECG

[HRJ+15] Alexander Hoffmann, Martin Rohrmüller, Anton Jesser, Ines dos Santos Vieira, Wolf Gero Schmidt, and Sonja Herres-Pawlis. Errata: Corrigendum: Geometrical and optical benchmarking of copper(II) guanidine–quinoline complexes: Insights from TD-DFT and many-body perturbation theory (Part II). *Journal of Computational Chemistry*, 36(4):272, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HRJ+14].

Hahnke:2010:PAS

[HRK+10] Volker Hähnke, Matthias Rupp, Mireille Krier, Friedrich Rippmann, and Gisbert Schneider. Pharmacophore alignment search tool: Influence of canonical atom labeling on similarity searching. *Journal of Computational Chemistry*, 31(15): 2810–2826, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2011:CSR

[HRL11] Wen-Fei Huang, P. Raghunath, and M. C. Lin. Computational study on the reactions of H_2O_2 on TiO_2 anatase (101) and rutile (110) surfaces. *Journal of Computational Chemistry*, 32(6):1065–1081, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hernandez-Rodriguez:2013:EDD

[HRMAL+13] Erix Wiliam Hernández-Rodríguez, Ana Lilian Montero-Alejo, Rafael López, Elsa Sánchez-García, Luis Alberto Montero-Cabrera, and José Manuel García de la Vega. Electron density deformations provide new insights into the spectral shift of rhodopsins. *Journal of Computational Chemistry*, 34(28):2460–2471, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hahnke:2011:PASb

[HS11] Volker Hähnke and Gisbert Schneider. Pharmacophore alignment search tool: Influence of scoring systems on text-based similarity searching. *Journal of Computational Chemistry*, 32 (8):1635–1647, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Helmich:2012:SRM

[HS12] Benjamin Helmich and Marek Sierka. Similarity recognition of molecular structures by optimal atomic matching and rotational superposition. *Journal of Computational Chemistry*, 33(2):134–140, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harris:2014:ISB

[HS14a] Travis V. Harris and Robert K. Szilagyi. Iron–sulfur bond covalency from electronic structure calculations for classical iron–sulfur clusters. *Journal of Computational Chemistry*, 35 (7):540–552, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2014:SCM

[HS14b] Hao Hu and Lin Shen. In silico concurrent multisite pH titration in proteins. *Journal of Computational Chemistry*, 35(20): 1491–1498, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hagras:2016:ETP

[HS16a] Muhammad A. Hagras and Alexei A. Stuchebrukhov. Electron tunneling in proteins program. *Journal of Computa-*

tional Chemistry, 37(15):1388–1395, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harris:2016:PEE

[HS16b] Travis V. Harris and Robert K. Szilagyi. Protein environmental effects on iron-sulfur clusters: a set of rules for constructing computational models for inner and outer coordination spheres. *Journal of Computational Chemistry*, 37(18): 1681–1696, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2017:SDS

[HS17a] Ryuhei Harada and Yasuteru Shigeta. Structural dissimilarity sampling with dynamically self-guiding selection. *Journal of Computational Chemistry*, 38(22):1921–1929, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2017:TSP

[HS17b] Ryuhei Harada and Yasuteru Shigeta. Temperature-shuffled parallel cascade selection molecular dynamics accelerates the structural transitions of proteins. *Journal of Computational Chemistry*, 38(31):2671–2674, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Heyndrickx:2011:PSB

[HSB+11] Wouter Heyndrickx, Pedro Salvador, Patrick Bultinck, Miquel Solà, and Eduard Matito. Performance of 3D-space-based atoms-in-molecules methods for electronic delocalization aromaticity indices. *Journal of Computational Chemistry*, 32(3): 386–395, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hanscam:2019:SSA

[HSB+19] Rebecca Hanscam, Eric M. Shepard, Joan B. Broderick, Valérie Copié, and Robert K. Szilagyi. Secondary structure analysis of peptides with relevance to iron-sulfur cluster nesting. *Journal of Computational Chemistry*, 40(2):515–526, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hellstrom:2015:TDE

[HSH15] Matti Hellström, Daniel Spångberg, and Kersti Hermansson. Treatment of delocalized electron transfer in periodic and embedded cluster DFT calculations: the case of Cu on ZnO $(10\bar{1}0)$. *Journal of Computational Chemistry*, 36(32):2394–2405, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haack:2018:DIB

[HSJ18] Rebekka Haack, Stephan Schulz, and Georg Jansen. Dispersion interactions between neighboring Bi atoms in $(BiH_3)_2$ and $Te(BiR_2)_2$. *Journal of Computational Chemistry*, 39(20): 1413–1423, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Han:2011:RRP

[HSL+11] Peipei Han, Kehe Su, Yan Liu, Yanli Wang, Xin Wang, Qingfeng Zeng, Laifei Cheng, and Litong Zhang. Reaction rate of propene pyrolysis. *Journal of Computational Chemistry*, 32(13):2745–2755, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayami:2014:EAC

[HSN14] Masao Hayami, Junji Seino, and Hiromi Nakai. Extension of accompanying coordinate expansion and recurrence relation method for general-contraction basis sets. *Journal of Computational Chemistry*, 35(20):1517–1527, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayami:2018:RLS

[HSN+18] Masao Hayami, Junji Seino, Yuya Nakajima, Masahiko Nakano, Yasuhiro Ikabata, Takeshi Yoshikawa, Takuro Oyama, Kenta Hiraga, So Hirata, and Hiromi Nakai. RAQET: Large-scale two-component relativistic quantum chemistry program package. *Journal of Computational Chemistry*, 39 (27):2333–2344, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hsu:2014:NPS

[Hsu14] Po-Jen Hsu. A new perspective of shape recognition to discover the phase transition of finite-size clusters. *Journal of Computational Chemistry*, 35(14):1082–1092, May 30, 2014.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

He:2019:EIG

[HSW+19] Gaoqi He, Yiping Song, Wenhao Wei, Xia Wang, Xingjian Lu, and Honglin Li. eSHAFTS: Integrated and graphical drug design software based on 3D molecular similarity. *Journal of Computational Chemistry*, 40(6):826–838, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hao:2011:ACV

[HSY+11] Qiang Hao, Andrew C. Simmonett, Yukio Yamaguchi, De-Cai Fang, and Henry F. Schaefer III. From acetylene complexes to vinylidene structures: The GeC_2H_2 system. *Journal of Computational Chemistry*, 32(1):15–22, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2011:IQD

[HSZ+11] Zhaowei Huang, Hui Sun, Houyu Zhang, Yue Wang, and Fei Li. π–π interaction of quinacridone derivatives. *Journal of Computational Chemistry*, 32(10):2055–2063, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2015:ECS

[HTS15] Ryuhei Harada, Yu Takano, and Yasuteru Shigeta. Enhanced conformational sampling method for proteins based on the TaBoo SeArch algorithm: Application to the folding of a mini-protein, chignolin. *Journal of Computational Chemistry*, 36 (10):763–772, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2017:CFP

[HTS17] Ryuhei Harada, Yu Takano, and Yasuteru Shigeta. Common folding processes of mini-proteins: Partial formations of secondary structures initiate the immediate protein folding. *Journal of Computational Chemistry*, 38(11):790–797, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higuchi:2019:MUA

[HTY19] Chisa Higuchi, Hiromasa Tanaka, and Kazunari Yoshizawa. Molecular understanding of the adhesive interactions between silica surface and epoxy resin: Effects of interfacial water. *Journal of Computational Chemistry*, 40(1):164–171, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2016:FSL

[Hua16] Bolong Huang. $4f$ fine-structure levels as the dominant error in the electronic structures of binary lanthanide oxides. *Journal of Computational Chemistry*, 37(9):825–835, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huggins:2012:BTA

[Hug12] David J. Huggins. Benchmarking the thermodynamic analysis of water molecules around a model beta sheet. *Journal of Computational Chemistry*, 33(15):1383–1392, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huggins:2014:CDM

[Hug14] David J. Huggins. Comparing distance metrics for rotation using the k-nearest neighbors algorithm for entropy estimation. *Journal of Computational Chemistry*, 35(5):377–385, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hunter:2012:DBS

[HvM12] Ruairidh S. Hunter and Tanja van Mourik. DNA base stacking: the stacked uracil/uracil and thymine/thymine minima. *Journal of Computational Chemistry*, 33(27):2161–2172, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hogan:2016:CBH

[HvM16] Simon W. L. Hogan and Tanja van Mourik. Competition between hydrogen and halogen bonding in halogenated 1-methyluracil:water systems. *Journal of Computational Chemistry*, 37(8):763–770, March 30, 2016. CODEN JCCHDD.

ISSN 0192-8651 (print), 1096-987X (electronic). See corrigendum [HvM17].

Hogan:2017:ECC

[HvM17] Simon W. L. Hogan and Tanja van Mourik. Erratum: Corrigendum: Competition between Hydrogen and Halogen Bonding in Halogenated 1-Methyluracil:Water Systems. *Journal of Computational Chemistry*, 38(12):933, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [HvM16].

Hogan:2019:HBM

[HvM19] Simon W. L. Hogan and Tanja van Mourik. Halogen bonding in mono- and dihydrated halobenzene. *Journal of Computational Chemistry*, 40(3):554–561, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hussain:2016:BAC

[HVS16] M. Althaf Hussain, Dolly Vijay, and G. Narahari Sastry. Buckybowls as adsorbents for CO_2, CH_4, and C_2H_2: Binding and structural insights from computational study. *Journal of Computational Chemistry*, 37(3):366–377, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hatanaka:2019:TSL

[HW19] Miho Hatanaka and Tomonari Wakabayashi. Theoretical study of lanthanide-based in vivo luminescent probes for detecting hydrogen peroxide. *Journal of Computational Chemistry*, 40(2):500–506, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hrovat:2019:CNP

[HWB19] David A. Hrovat, Xue-Bin Wang, and Weston Thatcher Borden. Calculations on 1,8-naphthoquinone predict that the ground state of this diradical is a singlet. *Journal of Computational Chemistry*, 40(1):119–126, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hou:2011:APM

[HWLW11] Tingjun Hou, Junmei Wang, Youyong Li, and Wei Wang. Assessing the performance of the molecular mechanics/Poisson

Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. *Journal of Computational Chemistry*, 32(5):866–877, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2016:QST

[HXM+16] Ming Xing Hu, Tianlv Xu, Roya Momen, Guo Huan, Steven R. Kirk, Samantha Jenkins, and Michael Filatov. A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. *Journal of Computational Chemistry*, 37(29):2588–2596, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2010:IPE

[HYD10] Zheng Guo Huang, Lei Yu, and Yu Mei Dai. An ab initio potential energy surface and vibrational energy levels of ZnH_2. *Journal of Computational Chemistry*, 31(5):986–993, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Han:2011:END

[HYL+11] Chong Han, Shi-Shen Yan, Xue-Ling Lin, Shu-Jun Hu, Ming-Wen Zhao, Xin-Xin Yao, Yan-Xue Chen, Guo-Lei Liu, and Liang-Mo Mei. Effect of native defects and Co doping on ferromagnetism in HfO_2: First-principles calculations. *Journal of Computational Chemistry*, 32(7):1298–1302, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoque:2016:SNU

[HYMZ16] Md Tamjidul Hoque, Yuedong Yang, Avdesh Mishra, and Yaoqi Zhou. Software news and updates: sDFIRE: Sequence-specific statistical energy function for protein structure prediction by decoy selections. *Journal of Computational Chemistry*, 37(12):1119–1124, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harada:2019:TPS

[HYNS19] Ryuhei Harada, Ryunosuke Yoshino, Hiroaki Nishizawa, and Yasuteru Shigeta. Temperature-pressure shuffling outlier flooding method enhances the conformational sampling of proteins. *Journal of Computational Chemistry*, 40(15):1530–1537, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirano:2019:DAF

[HYSF19] Ryosuke Hirano, Tsubasa Yabuchi, Minoru Sakurai, and Tadaomi Furuta. Development of an ATP force field for coarse-grained simulation of ATPases and its application to the maltose transporter. *Journal of Computational Chemistry*, 40(24):2096–2102, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hori:2011:FEP

[HYUS11] Kenji Hori, Toru Yamaguchi, Keita Uezu, and Michinori Sumimoto. A free-energy perturbation method based on Monte Carlo simulations using quantum mechanical calculations (QM/MC/FEP method): Application to highly solvent-dependent reactions. *Journal of Computational Chemistry*, 32(5):778–786, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hao:2013:CGB

[HYYZ13] Ge-Fei Hao, Sheng-Gang Yang, Guang-Fu Yang, and Chang-Guo Zhan. Computational gibberellin-binding channel discovery unraveling the unexpected perception mechanism of hormone signal by gibberellin receptor. *Journal of Computational Chemistry*, 34(24):2055–2064, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Han:2011:NQD

[HZ11] Boran Han and Yujun Zheng. Nonadiabatic quantum dynamics in $O(^3P) + H_2 \rightarrow OH + H$: a revisited study. *Journal of Computational Chemistry*, 32(16):3520–3525, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2013:NSD

[HZ13] Sheng-You Huang and Xiaoqin Zou. A nonredundant structure dataset for benchmarking protein-RNA computational docking. *Journal of Computational Chemistry*, 34(4):311–318, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2017:PES

[HZSS17] Zhubin Hu, Bin Zhou, Zhenrong Sun, and Haitao Sun. Prediction of excited-state properties of oligoacene crystals using polarizable continuum model-tuned range-separated hybrid functional approach. *Journal of Computational Chemistry*, 38(9):569–575, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

He:2010:GRP

[HZY+10] Ping-An He, Yan-Ping Zhang, Yu-Hua Yao, Yi-Fa Tang, and Xu-Ying Nan. The graphical representation of protein sequences based on the physicochemical properties and its applications. *Journal of Computational Chemistry*, 31(11):2136–2142, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ibrahim:2011:MMS

[Ibr11] Mahmoud A. A. Ibrahim. Molecular mechanical study of halogen bonding in drug discovery. *Journal of Computational Chemistry*, 32(12):2564–2574, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ibrahim:2017:ESM

[Ibr17] Ismail A. M. Ibrahim. Electronic structure, magnetic properties, and mixed valence character of $Ce_2Ni_3Si_5$ from first principles calculations. *Journal of Computational Chemistry*, 38 (29):2475–2480, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Illingworth:2012:SSS

[ICS+12] Christopher J. R. Illingworth, Sree V. Chintipalli, Stefano A. Serapian, Andrew D. Miller, Vaclav Veverka, Mark D. Carr, and Christopher A. Reynolds. The statistical significance of selected sense–antisense peptide interactions. *Journal of Computational Chemistry*, 33(16):1440–1447, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [ICS+13].

Illingworth:2013:ESS

[ICS+13] Christopher J. R. Illingworth, Sree V. Chintapalli, Stefano A. Serapian, Andrew D. Miller, Vaclav Veverka, Mark D. Carr, and Christopher A. Reynolds. Erratum: The statistical significance of selected sense–antisense peptide interactions [J. Comp. Chem. **33**, 1440–1447]. *Journal of Computational Chemistry*, 34(3):256, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [ICS+12].

Ioannidis:2016:SNU

[IGK16] Efthymios I. Ioannidis, Terry Z. H. Gani, and Heather J. Kulik. Software news and updates: molSimplify: a toolkit for automating discovery in inorganic chemistry. *Journal of Computational Chemistry*, 37(22):2106–2117, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iype:2013:PRF

[IHJ+13] E. Iype, M. Hütter, A. P. J. Jansen, S. V. Nedea, and C. C. M. Rindt. Parameterization of a reactive force field using a Monte Carlo algorithm. *Journal of Computational Chemistry*, 34 (13):1143–1154, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ihlenfeldt:2012:LEC

[Ihl12] Wolf-D. Ihlenfeldt. Letters to the editor: Comment on the paper "Indexing molecules with chemical graph identifiers' by Elisabeth Gregori-Puigjané, Rut Garriga-Sust, and Jordi Mestres. *Journal of Computational Chemistry*, 33(2): 237, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [GPGSM11] and response [GPGSM12].

Ito:2010:SFC

[II10] Yuko Ito and Mitsunori Ikeguchi. Structural fluctuation and concerted motions in F_1-ATPase: a molecular dynamics study. *Journal of Computational Chemistry*, 31(11):2175–2185, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ivanova:2018:TLM

[II18] Nikoleta Ivanova and Anela Ivanova. Testing the limits of model membrane simulations — bilayer composition and pressure scaling. *Journal of Computational Chemistry*, 39(8):387–396, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikegami:2010:FMO

[IIF+10] Tsutomu Ikegami, Toyokazu Ishida, Dmitri G. Fedorov, Kazuo Kitaura, Yuichi Inadomi, Hiroaki Umeda, Mitsuo Yokokawa, and Satoshi Sekiguchi. Fragment molecular orbital study of the electronic excitations in the photosynthetic reaction center of Blastochloris viridis. *Journal of Computational Chemistry*, 31(2):447–454, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishikura:2015:EEN

[IIHY15] Takakazu Ishikura, Yuki Iwata, Tatsuro Hatano, and Takahisa Yamato. Energy exchange network of inter-residue interactions within a thermally fluctuating protein molecule: a computational study. *Journal of Computational Chemistry*, 36 (22):1709–1718, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Imamura:2013:LCO

[IKN13] Yutaka Imamura, Rie Kobayashi, and Hiromi Nakai. Linearity condition for orbital energies in density functional theory (III): Benchmark of total energies. *Journal of Computational Chemistry*, 34(14):1218–1225, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iliff:2011:POA

[ILKR11] Hadley A. Iliff, Diane L. Lynch, Evangelia Kotsikorou, and Patricia H. Reggio. Parameterization of Org27569: an allosteric modulator of the cannabinoid CB_1G protein-coupled receptor. *Journal of Computational Chemistry*, 32(10):2119–2126, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishizuka:2017:ECI

[IM17] Ryosuke Ishizuka and Nobuyuki Matubayasi. Effective charges of ionic liquid determined self-consistently through combination of molecular dynamics simulation and density-functional theory. *Journal of Computational Chemistry*, 38 (30):2559–2569, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iida:2016:VFE

[IMK+16] Shinji Iida, Tadaaki Mashimo, Takashi Kurosawa, Hironobu Hojo, Hiroya Muta, Yuji Goto, Yoshifumi Fukunishi, Haruki Nakamura, and Junichi Higo. Variation of free-energy landscape of the p53 C-terminal domain induced by acetylation: Enhanced conformational sampling. *Journal of Computational Chemistry*, 37(31):2687–2700, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ignjatovic:2018:CMG

[IMSR18] Majda Misini Ignjatović, Paulius Mikulskis, Pär Söderhjelm, and Ulf Ryde. Can MM/GBSA calculations be sped up by system truncation? *Journal of Computational Chemistry*, 39 (7):361–372, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishikawa:2013:XOA

[IN13] Atsushi Ishikawa and Hiroshi Nakatsuji. XPS of oxygen atoms on Ag(111) and Ag(110) surfaces: Accurate study with SAC/SAC-CI combined with dipped adcluster model. *Journal of Computational Chemistry*, 34(21):1828–1834, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inagaki:2019:EPE

[IN19] Taichi Inagaki and Masataka Nagaoka. Electrode polarization effects on interfacial kinetics of ionic liquid at graphite surface: an extended Lagrangian-based constant potential molecular dynamics simulation study. *Journal of Computational Chemistry*, 40(24):2131–2145, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Imada:2018:DFS

[INT18] Yasuhiro Imada, Haruki Nakamura, and Yu Takano. Density functional study of porphyrin distortion effects on redox potential of heme. *Journal of Computational Chemistry*, 39(3): 143–150, January 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Itoh:2013:CRE

[IO13a] Satoru G. Itoh and Hisashi Okumura. Coulomb replica-exchange method: Handling electrostatic attractive and repulsive forces for biomolecules. *Journal of Computational Chemistry*, 34(8):622–639, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Itoh:2013:HRP

[IO13b] Satoru G. Itoh and Hisashi Okumura. Hamiltonian replica-permutation method and its applications to an alanine dipeptide and amyloid-β (29–42) peptides. *Journal of Computational Chemistry*, 34(29):2493–2497, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Izanloo:2011:DDD

[IPAA11] C. Izanloo, G. A. Parsafar, H. Abroshan, and H. Akbarzadeh. Denaturation of Drew–Dickerson DNA in a high salt concentration medium: Molecular dynamics simulations. *Journal of Computational Chemistry*, 32(16):3354–3361, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishida:2010:BMH

[Ish10] Hisashi Ishida. Branch migration of Holliday junction in RuvA tetramer complex studied by umbrella sampling simulation using a path-search algorithm. *Journal of Computational Chemistry*, 31(12):2317–2329, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishida:2012:FTG

[Ish12] Kazuhiro Ishida. Fourier transform general formula for systematic potentials. *Journal of Computational Chemistry*, 33 (9):924–936, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikebe:2014:ALS

[ISK14] Jinzen Ikebe, Shun Sakuraba, and Hidetoshi Kono. Adaptive lambda square dynamics simulation: an efficient conformational sampling method for biomolecules. *Journal of Computational Chemistry*, 35(1):39–50, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishikawa:2018:RMC

[ISM18] Takeshi Ishikawa, Kota Sakakura, and Yuji Mochizuki. RI-MP3 calculations of biomolecules based on the fragment molecular orbital method. *Journal of Computational Chemistry*, 39(24):1970–1978, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Imamura:2013:KED

[ISN13] Yutaka Imamura, Jun Suzuki, and Hiromi Nakai. Kinetic energy decomposition scheme based on information theory. *Journal of Computational Chemistry*, 34(32):2787–2795, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inui:2013:FFM

[ISO+13] Tomoya Inui, Yasuteru Shigeta, Katsuki Okuno, Takeshi Baba, Ryohei Kishi, and Masayoshi Nakano. Finite-field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an open-shell singlet molecule in solvents. *Journal of Computational Chemistry*, 34 (27):2345–2352, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Illingworth:2010:CBS

[ISP+10] Christopher J. R. Illingworth, Paul D. Scott, Kevin E. B. Parkes, Christopher R. Snell, Matthew P. Campbell, and Christopher A. Reynolds. Connectivity and binding-site recognition: Applications relevant to drug design. *Journal of Computational Chemistry*, 31(15):2677–2688, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishikawa:2019:REB

[IT19] Atsushi Ishikawa and Yoshitaka Tateyama. Reaction energy benchmarks of hydrocarbon combustion by Gaussian basis and plane wave basis approaches. *Journal of Computational Chemistry*, 40(20):1866–1873, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikabata:2015:LRD

[ITIN15] Yasuhiro Ikabata, Yusuke Tsukamoto, Yutaka Imamura, and Hiromi Nakai. Local response dispersion method in periodic systems: Implementation and assessment. *Journal of Computational Chemistry*, 36(5):303–311, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iioka:2019:KSL

[ITY+19] Tatsuya Iioka, Satoshi Takahashi, Yuichiro Yoshida, Yoshihiro Matsumura, Shuichi Hiraoka, and Hirofumi Sato. A kinetics study of ligand substitution reaction on dinuclear platinum complexes: Stochastic versus deterministic approach. *Journal of Computational Chemistry*, 40(1):279–285, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ikebe:2011:TTT

[IUK+11] Jinzen Ikebe, Koji Umezawa, Narutoshi Kamiya, Takanori Sugihara, Yasushige Yonezawa, Yu Takano, Haruki Nakamura, and Junichi Higo. Theory for trivial trajectory parallelization of multicanonical molecular dynamics and application to a polypeptide in water. *Journal of Computational Chemistry*, 32(7):1286–1297, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inakollu:2018:SBC

[IY18] V. S. Sandeep Inakollu and Haibo Yu. A systematic benchmarking of computational vibrational spectroscopy with DFTB3: Normal mode analysis and Fast Fourier Transform dipole autocorrelation function. *Journal of Computational Chemistry*, 39(25):2067–2078, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inagaki:2011:PCE

[IYK11] Taichi Inagaki, Takeshi Yamamoto, and Shigeki Kato. Proton-coupled electron transfer of the phenoxyl/phenol couple: Effect of Hartree–Fock exchange on transition structures. *Journal of Computational Chemistry*, 32(14):3081–3091, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jalili:2010:MDS

[JA10] S. Jalili and M. Akhavan. Molecular dynamics simulation study of association in trifluoroethanol/water mixtures. *Journal of Computational Chemistry*, 31(2):286–294, January 30,

2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2014:RBS

[Jab14] Mirosław Jabłoński. Red and blue shifted hydridic bonds. *Journal of Computational Chemistry*, 35(24):1739–1747, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2018:BPB

[Jab18a] Miroslaw Jabloński. Bond paths between distant atoms do not necessarily indicate dominant interactions. *Journal of Computational Chemistry*, 39(26):2183–2195, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2018:HTB

[Jab18b] Miroslaw Jabloński. Hydride-triel Bonds. *Journal of Computational Chemistry*, 39(19):1177–1191, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2017:EMI

[JAH+17] Zhe Jia, Christine Ackroyd, Tingting Han, Vibhor Agrawal, Yinling Liu, Kenneth Christensen, and Brian Dominy. Effects from metal ion in tumor endothelial marker 8 and anthrax protective antigen: BioLayer Interferometry experiment and molecular dynamics simulation study. *Journal of Computational Chemistry*, 38(15):1183–1190, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jayasinghe-Arachchige:2019:HCD

[JAHS+19] Vindi M. Jayasinghe-Arachchige, Qiaoyu Hu, Gaurav Sharma, Thomas J. Paul, Marcus Lundberg, David Quinonero, Tatjana N. Parac-Vogt, and Rajeev Prabhakar. Hydrolysis of chemically distinct sites of human serum albumin by polyoxometalate: a hybrid QM/ MM (ONIOM) study. *Journal of Computational Chemistry*, 40(1):51–61, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Janesko:2016:TAE

[Jan16] Benjamin G. Janesko. Topological analysis of the electron delocalization range. *Journal of Computational Chemistry*, 37

(21):1993–2005, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jacob:2011:DAP

[JBAM11] Reed B. Jacob, Casey W. Bullock, Tim Andersen, and Owen M. McDougal. DockoMatic: Automated peptide analog creation for high throughput virtual screening. *Journal of Computational Chemistry*, 32(13):2936–2941, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jacob:2011:PSF

[JBB+11] Christoph R. Jacob, S. Maya Beyhan, Rosa E. Bulo, André Severo Pereira Gomes, Andreas W. Götz, Karin Kiewisch, Jetze Sikkema, and Lucas Visscher. PyADF — a scripting framework for multiscale quantum chemistry. *Journal of Computational Chemistry*, 32(10):2328–2338, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jaramillo-Botero:2011:LSL

[JBSQG11] Andres Jaramillo-Botero, Julius Su, An Qi, and William A. Goddard III. Large-scale, long-term nonadiabatic electron molecular dynamics for describing material properties and phenomena in extreme environments. *Journal of Computational Chemistry*, 32(3):497–512, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2016:NHR

[JC16] Zhiguang Jia and Jianhan Chen. Necessity of high-resolution for coarse-grained modeling of flexible proteins. *Journal of Computational Chemistry*, 37(18):1725–1733, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ji:2010:KMH

[JCG+10] Yue-Meng Ji, Fenglei Cao, Hui Gao, Xiangzhi Li, Cunyuan Zhao, Chengyong Su, Jing-Yao Liu, and Ze-Sheng Li. On the kinetic mechanism of the hydrogen abstraction reactions of the hydroxyl radical with CH_3CF_2Cl and CH_3CFCl_2: a dual level direct dynamics study. *Journal of Computational Chemistry*, 31(3):510–519, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jing:2011:GMM

[JCG+11] Qun Jing, Hai-Bin Cao, Gui-Xian Ge, Yuan Xu Wang, Hong-Xia Yan, Zi-Ying Zhang, and Yun-Hu Liu. Giant magnetic moment of the core-shell Co_{13} @Mn_{20} clusters: First-principles calculations. *Journal of Computational Chemistry*, 32(11):2474–2478, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jurinovich:2018:SNU

[JCGM18] Sandro Jurinovich, Lorenzo Cupellini, Ciro A. Guido, and Benedetta Mennucci. Software news and updates: EXAT: EXcitonic Analysis Tool. *Journal of Computational Chemistry*, 39(5):279–286, February 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jara-Cortes:2017:CBE

[JCGVPHT17] Jesús Jara-Cortés, José Manuel Guevara-Vela, Ángel Martín Pendás, and Jesús Hernández-Trujillo. Chemical bonding in excited states: Energy transfer and charge redistribution from a real space perspective. *Journal of Computational Chemistry*, 38(13):957–970, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jara-Cortes:2018:EAC

[JCHT18] Jesús Jara-Cortés and Jesús Hernández-Trujillo. Energetic Analysis of Conjugated Hydrocarbons Using the Interacting Quantum Atoms Method. *Journal of Computational Chemistry*, 39(18):1103–1111, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jo:2017:RCG

[JCL+17] Sunhwan Jo, Xi Cheng, Jumin Lee, Seonghoon Kim, Sang-Jun Park, Dhilon S. Patel, Andrew H. Beaven, Kyu Il Lee, Huan Rui, Soohyung Park, Hui Sun Lee, Benoît Roux, Alexander D. MacKerell, Jr., Jeffrey B. Klauda, Yifei Qi, and Wonpil Im. Review: CHARMM–GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, 38(15): 1114–1124, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jahangiri:2014:PDF

[JCP14] Soran Jahangiri, Lemin Cai, and Gilles H. Peslherbe. Performance of density-functional tight-binding models in describing hydrogen-bonded anionic-water clusters. *Journal of Computational Chemistry*, 35(23):1707–1715, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jaillet:2011:RTC

[JCPC11] Léonard Jaillet, Francesc J. Corcho, Juan-Jesús Pérez, and Juan Cortés. Randomized tree construction algorithm to explore energy landscapes. *Journal of Computational Chemistry*, 32(16):3464–3474, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2010:INA

[JCX10] Xuewei Jiang, Changjun Chen, and Yi Xiao. Improvements of network approach for analysis of the folding free-energy surface of peptides and proteins. *Journal of Computational Chemistry*, 31(13):2502–2509, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jones:2019:CAU

[JDW+19] Walker M. Jones, Aaron G. Davis, R. Hunter Wilson, Katherine L. Elliott, and Isaiah Sumner. A conserved asparagine in a ubiquitin-conjugating enzyme positions the substrate for nucleophilic attack. *Journal of Computational Chemistry*, 40 (22):1969–1977, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jorge:2017:PHSa

[JGS+17] Miguel Jorge, Nuno M. Garrido, Carlos J. V. Simões, Cândida G. Silva, and Rui M. M. Brito. Predicting hydrophobic solvation by molecular simulation: 1. Testing united-atom alkane models. *Journal of Computational Chemistry*, 38(6): 346–358, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jenkins:2013:SNU

[JHH+13] David D. Jenkins, Jason B. Harris, Elizabeth E. Howell, Robert J. Hinde, and Jerome Baudry. Software news and updates: STAAR: Statistical analysis of aromatic rings. *Journal* of *Computational Chemistry*, 34(6):518–522, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jimenez-Halla:2009:TAT

[JHMB+09] J. Oscar C. Jiménez-Halla, Eduard Matito, Lluís Blancafort, Juvencio Robles, and Miquel Solà. Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. *Journal of Computational Chemistry*, 30(16):2764–2776, December 2009. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [JHMB+11].

Jimenez-Halla:2011:ETA

[JHMB+11] J. Oscar C. Jiménez-Halla, Eduard Matito, Lluís Blancafort, Juvencio Robles, and Miquel Solà. Erratum: "Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts". *Journal of Computational Chemistry*, 32 (2):372–373, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [JHMB+09].

Jia:2019:SFE

[Jia19] Xiangyu Jia. Solvation free energy calculations: The combination between the implicitly polarized fixed-charge model and the reference potential strategy. *Journal of Computational Chemistry*, 40(32):2801–2809, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jakobtorweihen:2013:CCM

[JIS13] Sven Jakobtorweihen, Thomas Ingram, and Irina Smirnova. Combination of COSMOmic and molecular dynamics simulations for the calculation of membrane-water partition coefficients. *Journal of Computational Chemistry*, 34(15):1332–1340, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiao:2016:CCS

[JJAB16] Haijun Jiao, Kathrin Junge, Elisabetta Alberico, and Matthias Beller. A comparative computationally study about the defined m(II) pincer hydrogenation catalysts (m = fe, ru, os). *Journal of Computational Chemistry*, 37(2):168–176, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jin:2013:CPR

[JJH+13] Yingdi Jin, Erin R. Johnson, Xiangqian Hu, Weitao Yang, and Hao Hu. Contributions of Pauli repulsions to the energetics and physical properties computed in QM/MM methods. *Journal of Computational Chemistry*, 34(27):2380–2388, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Joy:2016:CXZ

[JJJ16] Jyothish Joy, Anex Jose, and Eluvathingal D. Jemmis. Continuum in the X–Z—Y weak bonds: Z = main group elements. *Journal of Computational Chemistry*, 37(2):270–279, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jeong:2014:SNU

[JJW+14] Jong Cheol Jeong, Sunhwan Jo, Emilia L. Wu, Yifei Qi, Viviana Monje-Galvan, Min Sun Yeom, Lev Gorenstein, Feng Chen, Jeffery B. Klauda, and Wonpil Im. Software news and updates: ST-analyzer: a Web-based user interface for simulation trajectory analysis. *Journal of Computational Chemistry*, 35(12):957–963, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jankowska:2016:SOZ

[JKS+16] Marzena Jankowska, Teobald Kupka, Leszek Stobiński, Rasmus Faber, Evanildo G. Lacerda Jr., and Stephan P. A. Sauer. Spin-orbit ZORA and four-component Dirac–Coulomb estimation of relativistic corrections to isotropic nuclear shieldings and chemical shifts of noble gas dimers. *Journal of Computational Chemistry*, 37(4):395–403, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Joshi:2019:DPP

[JL19] Dhananjay C. Joshi and Jung-Hsin Lin. Delineating protein–protein curvilinear dissociation pathways and energetics with naïve multiple-walker umbrella sampling simulations. *Journal of Computational Chemistry*, 40(17):1652–1663, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2017:SNU

[JLCA17] Zhe Jia, Lin Li, Arghya Chakravorty, and Emil Alexov. Software news and updates: Treating ion distribution with Gaussian-based smooth dielectric function in DelPhi. *Journal of Computational Chemistry*, 38(22):1974–1979, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2014:SCH

[JLH+14] Shuai Jiang, Yi-Rong Liu, Teng Huang, Hui Wen, Kang-Ming Xu, Wei-Xiong Zhao, Wei-Jun Zhang, and Wei Huang. Study of Cl^- $(H_2O)_n$ (n = 1–4) using basin-hopping method coupled with density functional theory. *Journal of Computational Chemistry*, 35(2):159–165, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2019:EES

[JLLW19] Qingqing Jia, Hai-Bei Li, Mo Luo, and Jingjing Wang. Effects of electronic structure of adjacent carbon on the strength of C-F$\cdots$H-F organofluorine hydrogen bonds. *Journal of Computational Chemistry*, 40(28):2473–2481, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2010:CSM

[JLS+10] Xiu-Juan Jia, You-Jun Liu, Jing-Yu Sun, Hao Sun, Fang Wang, Zhong-Min Su, Xiu-Mei Pan, and Rong-Shun Wang. Computational studies on the mechanism and kinetics of Cl reaction with C_2H_5I. *Journal of Computational Chemistry*, 31 (12):2263–2272, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Johnson:2018:CAT

[JLS18] Quentin R. Johnson, Richard J. Lindsay, and Tongye Shen. CAMERRA: an analysis tool for the computation of conformational dynamics by evaluating residue-residue associations. *Journal of Computational Chemistry*, 39(20):1568–1578, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jadraque:2011:CTP

[JM11] Maria Jadraque and Margarita Martin. Charge-transfer processes in the assembly of Si_n O_m neutral clusters. *Journal of Computational Chemistry*, 32(16):3497–3504, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jambeck:2013:PAC

[JMLL13] Joakim P. M. Jämbeck, Francesca Mocci, Alexander P. Lyubartsev, and Aatto Laaksonen. Partial atomic charges and their impact on the free energy of solvation. *Journal of Computational Chemistry*, 34(3):187–197, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2013:ELT

[JMS13] Jaewoon Jung, Takaharu Mori, and Yuji Sugita. Efficient lookup table using a linear function of inverse distance squared. *Journal of Computational Chemistry*, 34(28):2412–2420, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2014:MCM

[JMS14] Jaewoon Jung, Takaharu Mori, and Yuji Sugita. Midpoint cell method for hybrid (MPI + OpenMP) parallelization of molecular dynamics simulations. *Journal of Computational Chemistry*, 35(14):1064–1072, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiajun:2016:STQ

[JMX+16] D. Jiajun, J. R. Maza, Y. Xu, T. Xu, R. Momen, S. R. Kirk, and S. Jenkins. A stress tensor and QTAIM perspective on the substituent effects of biphenyl subjected to torsion. *Journal of Computational Chemistry*, 37(28):2508–2517, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2019:SMD

[JND+19] Jaewoon Jung, Wataru Nishima, Marcus Daniels, Gavin Bascom, Chigusa Kobayashi, Adetokunbo Adedoyin, Michael Wall, Anna Lappala, Dominic Phillips, William Fischer, Chang-Shung Tung, Tamar Schlick, Yuji Sugita, and

Karissa Y. Sanbonmatsu. Scaling molecular dynamics beyond 100,000 processor cores for large-scale biophysical simulations. *Journal of Computational Chemistry*, 40(21):1919–1930, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jorge:2017:PHSb

[Jor17] Miguel Jorge. Predicting hydrophobic solvation by molecular simulation: 2. New united-atom model for alkanes, alkenes, and alkynes. *Journal of Computational Chemistry*, 38(6):359–369, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jurij:2015:SNU

[JP15] Reščič Jurij and Linse Per. Software news and updates: MOLSIM: a modular molecular simulation software. *Journal of Computational Chemistry*, 36(16):1259–1274, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jesser:2014:GOB

[JRSHP14] Anton Jesser, Martin Rohrmüller, Wolf Gero Schmidt, and Sonja Herres-Pawlis. Geometrical and optical benchmarking of copper guanidine–quinoline complexes: Insights from TD-DFT and many-body perturbation theory. *Journal of Computational Chemistry*, 35(1):1–17, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jerbi:2017:CSR

[JS17a] Jihène Jerbi and Michael Springborg. Computational study of the reactivity of cytosine derivatives. *Journal of Computational Chemistry*, 38(14):1049–1056, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2017:MPM

[JS17b] Jaewoon Jung and Yuji Sugita. Multiple program/multiple data molecular dynamics method with multiple time step integrator for large biological systems. *Journal of Computational Chemistry*, 38(16):1410–1418, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jo:2011:GRA

[JSD+11] Sunhwan Jo, Kevin C. Song, Heather Desaire, Alexander D. MacKerell Jr., and Wonpil Im. Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. *Journal of Computational Chemistry*, 32(14):3135–3141, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jerabek:2019:DES

[JSF19] Paul Jerabek, Peter Schwerdtfeger, and Gernot Frenking. Dative and electron-sharing bonding in transition metal compounds. *Journal of Computational Chemistry*, 40(1):247–264, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2010:SRP

[JSW10] Xiao-Nan Jiang, Chang-Liang Sun, and Chang-Sheng Wang. A scheme for rapid prediction of cooperativity in hydrogen bond chains of formamides, acetamides, and *N*-methylformamides. *Journal of Computational Chemistry*, 31 (7):1410–1420, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jin:2016:SCF

[JSXH16] Yingdi Jin, Neil Qiang Su, Xin Xu, and Hao Hu. Self-consistent field for fragmented quantum mechanical model of large molecular systems. *Journal of Computational Chemistry*, 37(3):321–326, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Johnson:2018:HBM

[JT18] Sarah N. Johnson and Gregory S. Tschumper. Hydrogen bonding in the mixed HF/HCl dimer: Is it better to give or receive? *Journal of Computational Chemistry*, 39(14):839–843, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jorgensen:2012:LEC

[JW12] Kameron R. Jorgensen and Angela K. Wilson. Letters to the editor: Comment on the paper “Extensive Theoretical Studies of a New Energetic Material: Tetrazino-Tetrazine-Tetraoxide (TTTO)” by Xinli Song, Jicun Li, Hua Hou, and

Baoshan Wang. *Journal of Computational Chemistry*, 33(24): 1967–1968, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SLHW09].

Jones:2016:MHD

[JW16] Leighton Jones and Benjamin J. Whitaker. Modeling a halogen dance reaction mechanism: a density functional theory study. *Journal of Computational Chemistry*, 37(18):1697–1703, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jensen:2015:ETS

[JWO15] Benjamin D. Jensen, Kristopher E. Wise, and Gregory M. Odegard. The effect of time step, thermostat, and strain rate on ReaxFF simulations of mechanical failure in diamond, graphene, and carbon nanotube. *Journal of Computational Chemistry*, 36(21):1587–1596, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jono:2010:MIQ

[JWST10] Ryota Jono, Yuusuke Watanabe, Kentaro Shimizu, and Tohru Terada. Multicanonical ab inito QM/MM molecular dynamics simulation of a peptide in an aqueous environment. *Journal of Computational Chemistry*, 31(6):1168–1175, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ji:2015:IBL

[JXSW15] Wen-Xin Ji, Wei Xu, W. H. Eugen Schwarz, and Shu-Guang Wang. Ionic bonding of lanthanides, as influenced by d- and f-atomic orbitals, by core-shells and by relativity. *Journal of Computational Chemistry*, 36(7):449–458, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jin:2016:HAT

[JYC+16] Zhao Jin, Chunwei Yang, Fenglei Cao, Feng Li, Zhifeng Jing, Long Chen, Zhe Shen, Liang Xin, Sijia Tong, and Huai Sun. Hierarchical atom type definitions and extensible all-atom force fields. *Journal of Computational Chemistry*, 37(7):653–664, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jungsuttiwong:2012:ECS

[JYS+12] Siriporn Jungsuttiwong, Thanisorn Yakhanthip, Yaowarat Surakhot, Janeeya Khunchalee, Taweesak Sudyoadsuk, Vinich Promarak, Nawee Kungwan, and Supawadee Namuangruk. The effect of conjugated spacer on novel carbazole derivatives for dye-sensitized solar cells: Density functional theory/ time-dependent density functional theory study. *Journal of Computational Chemistry*, 33(17):1517–1523, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ji:2012:EIP

[JZ12] Chang G. Ji and John Z. H. Zhang. Effect of interprotein polarization on protein–protein binding energy. *Journal of Computational Chemistry*, 33(16):1416–1420, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jafari:2017:RER

[JZ17] Mina Jafari and Paul M. Zimmerman. Reliable and efficient reaction path and transition state finding for surface reactions with the growing string method. *Journal of Computational Chemistry*, 38(10):645–658, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Johnston:2017:SDA

[JZL+17] Travis Johnston, Boyu Zhang, Adam Liwo, Silvia Crivelli, and Michela Taufer. In situ data analytics and indexing of protein trajectories. *Journal of Computational Chemistry*, 38 (16):1419–1430, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2014:AAP

[JZZM14] Xiangyu Jia, Juan Zeng, John Z. H. Zhang, and Ye Mei. Accessing the applicability of polarized protein-specific charge in linear interaction energy analysis. *Journal of Computational Chemistry*, 35(9):737–747, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kunz:2012:SNU

[KAG+12] Anna-Pitschna E. Kunz, Jane R. Allison, Daan P. Geerke, Bruno A. C. Horta, Philippe H. Hünenberger, Sereina Riniker, Nathan Schmid, and Wilfred F. van Gunsteren. Software news and updates: New functionalities in the GROMOS biomolecular simulation software. *Journal of Computational Chemistry*, 33(3):340–353, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kantardjiev:2015:SNU

[Kan15] Alexander A. Kantardjiev. Software news and updates: irGPU.proton.Net: Irregular strong charge interaction networks of protonatable groups in protein molecules — a GPU solver using the fast multipole method and statistical thermodynamics. *Journal of Computational Chemistry*, 36(9): 689–693, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koley:2012:CIC

[KAR12] D. Koley, E. Arunan, and S. Ramakrishnan. Computational investigations on covalent dimerization/oligomerization of polyacenes: Is it relevant to soot formation? *Journal of Computational Chemistry*, 33(21):1762–1772, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karton:2017:HRD

[Kar17] Amir Karton. How reliable is DFT in predicting relative energies of polycyclic aromatic hydrocarbon isomers? Comparison of functionals from different rungs of Jacob's ladder. *Journal of Computational Chemistry*, 38(6):370–382, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kawamura:2014:QCA

[KASH14] Toshiaki Kawamura, Minori Abe, Masaichi Saito, and Masahiko Hada. Quantum-chemical analyses of aromaticity, UV spectra, and NMR chemical shifts in plumbacyclopentadienylidenes stabilized by Lewis bases. *Journal of Computational Chemistry*, 35(11):847–853, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kang:2010:ADF

[KB10] Young Kee Kang and Byung Jin Byun. Assessment of density functionals with long-range and/or empirical dispersion corrections for conformational energy calculations of peptides.

Journal of Computational Chemistry, 31(16):2915–2923, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knight:2011:AEI

[KB11a] Jennifer L. Knight and Charles L. Brooks III. Applying efficient implicit nongeometric constraints in alchemical free energy simulations. *Journal of Computational Chemistry*, 32 (16):3423–3432, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knight:2011:SIS

[KB11b] Jennifer L. Knight and Charles L. Brooks III. Surveying implicit solvent models for estimating small molecule absolute hydration free energies. *Journal of Computational Chemistry*, 32(13):2909–2923, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Konig:2011:NBS

[KB11c] Gerhard König and Stefan Boresch. Non-Boltzmann sampling and Bennett's acceptance ratio method: How to profit from bending the rules. *Journal of Computational Chemistry*, 32 (6):1082–1090, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kazaryan:2013:ADF

[KB13] Andranik Kazaryan and Evert Jan Baerends. Assessment of density functional methods for reaction energetics: Iridium-catalyzed water oxidation as case study. *Journal of Computational Chemistry*, 34(10):870–878, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kessler:2014:MDH

[KB14a] Jiří Kessler and Petr Bouř. Molecular dynamics with helical periodic boundary conditions. *Journal of Computational Chemistry*, 35(21):1552–1559, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krause:2014:CLS

[KB14b] Katharina Krause and Thomas Bredow. Conductor-like screening model for relaxed excited states: Implementation in the semiempirical method MSINDO. *Journal of Computational Chemistry*, 35(7):553–564, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kendrick:2016:SNU

[KB16] John Kendrick and Andrew D. Burnett. Software news and updates: PDielec: the calculation of infrared and terahertz absorption for powdered crystals. *Journal of Computational Chemistry*, 37(16):1491–1504, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kolokathis:2019:KRC

[KB19] Panagiotis D. Kolokathis and Oleg M. Braun. KoBra: a rate constant method for prediction of the diffusion of sorbates inside nanoporous materials at different loadings. *Journal of Computational Chemistry*, 40(23):2053–2066, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalugina:2012:SHV

[KBC12] Yulia N. Kalugina, Mikhail A. Buldakov, and Victor N. Cherepanov. Static hyperpolarizability of the van der Waals complex CH_4N_2. *Journal of Computational Chemistry*, 33(32):2544–2553, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalyaanamoorthy:2013:LRM

[KC13a] Subha Kalyaanamoorthy and Yi-Ping Phoebe Chen. Ligand release mechanisms and channels in histone deacetylases. *Journal of Computational Chemistry*, 34(26):2270–2283, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaushik:2013:SDS

[KC13b] Ananth P. Kaushik and Paulette Clancy. Solvent-driven symmetry of self-assembled nanocrystal superlattices — a computational study. *Journal of Computational Chemistry*, 34(7):523–532, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koes:2014:SBV

[KC14] David Ryan Koes and Carlos J. Camacho. Shape-based virtual screening with volumetric aligned molecular shapes.

Journal of Computational Chemistry, 35(25):1824–1834, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalugina:2012:TIE

[KCB+12] Yulia N. Kalugina, Victor N. Cherepanov, Mikhail A. Buldakov, Natalia Zvereva-Loëte, and Vincent Boudon. Theoretical investigation of the ethylene dimer: Interaction energy and dipole moment. *Journal of Computational Chemistry*, 33(3):319–330, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Keceli:2018:SSM

[KCC+18] Murat Keçeli, Fabiano Corsetti, Carmen Campos, Jose E. Roman, Hong Zhang, Álvaro Vázquez-Mayagoitia, Peter Zapol, and Albert F. Wagner. SIESTA–SIPs: Massively parallel spectrum-slicing eigensolver for an ab initio molecular dynamics package. *Journal of Computational Chemistry*, 39 (22):1806–1814, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karilainen:2015:VWI

[KCK+15] Topi Karilainen, Oana Cramariuc, Mikael Kuisma, Kirsi Tappura, and Terttu I. Hukka. van der Waals interactions are critical in Car–Parrinello molecular dynamics simulations of porphyrin–fullerene dyads. *Journal of Computational Chemistry*, 36(9):612–621, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karczynska:2017:EMQ

[KCK+17] Agnieszka S. Karczyńska, Cezary Czaplewski, Paweł Krupa, Magdalena A. Mozolewska, Keehyoung Joo, Jooyoung Lee, and Adam Liwo. Ergodicity and model quality in template-restrained canonical and temperature/Hamiltonian replica exchange coarse-grained molecular dynamics simulations of proteins. *Journal of Computational Chemistry*, 38(31):2730–2746, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kurnosov:2014:EIP

[KCL+14] Alexander Kurnosov, Mario Cacciatore, Antonio Laganà, Fernando Pirani, Massimiliano Bartolomei, and Ernesto Garcia.

The effect of the intermolecular potential formulation on the state-selected energy exchange rate coefficients in N_2–N_2 collisions. *Journal of Computational Chemistry*, 35(9):722–736, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kopitz:2012:ISR

[KCPMG12] Hannes Kopitz, Daniel A. Cashman, Stefania Pfeiffer-Marek, and Holger Gohlke. Influence of the solvent representation on vibrational entropy calculations: Generalized Born versus distance-dependent dielectric model. *Journal of Computational Chemistry*, 33(9):1004–1013, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalita:2010:ACO

[KD10] Bulumoni Kalita and Ramesh C. Deka. Adsorption of CO on oxygen preadsorbed neutral and charged gas phase Pd_4 clusters: a density functional study. *Journal of Computational Chemistry*, 31(13):2476–2482, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klamt:2018:RCC

[KD18] Andreas Klamt and Michael Diedenhofen. A refined cavity construction algorithm for the conductor-like screening model. *Journal of Computational Chemistry*, 39(21):1648–1655, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kessler:2013:PVS

[KDB13] Jiří Kessler, Martin Dračínský, and Petr Bouř. Parallel variable selection of molecular dynamics clusters as a tool for calculation of spectroscopic properties. *Journal of Computational Chemistry*, 34(5):366–371, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kholod:2018:SNU

[KDR+18] Yana Kholod, Michael DeFilippo, Brittany Reed, Danielle Valdez, Grant Gillan, and Dmytro Kosenkov. Software news and updates: Excitation energy transfer pathways in light-harvesting proteins: Modeling with PyFREC. *Journal of Computational Chemistry*, 39(8):438–449, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2017:CBD

[KDS17] Anand Kumar, Miquel Duran, and Miquel Solà. Is coronene better described by Clar's aromatic π-sextet model or by the AdNDP representation? *Journal of Computational Chemistry*, 38(18):1606–1611, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Konc:2012:SNU

[KDT+12] Janez Konc, Matjaž Depolli, Roman Trobec, Kati Rozman, and Dušanka Janežič. Software news and updates: Parallel-ProBiS: Fast parallel algorithm for local structural comparison of protein structures and binding sites. *Journal of Computational Chemistry*, 33(27):2199–2203, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khanjari:2017:ANB

[KEMP17] Neda Khanjari, Hossein Eslami, and Florian Müller-Plathe. Adaptive-numerical-bias metadynamics. *Journal of Computational Chemistry*, 38(31):2721–2729, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kingsley:2016:RPP

[KERY+16] Laura J. Kingsley, Juan Esquivel-Rodríguez, Ying Yang, Daisuke Kihara, and Markus A. Lill. Ranking protein–protein docking results using steered molecular dynamics and potential of mean force calculations. *Journal of Computational Chemistry*, 37(20):1861–1865, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kobayashi:2018:AEC

[KFT18] Masato Kobayashi, Toshikazu Fujimori, and Tetsuya Taketsugu. Automated error control in divide-and-conquer self-consistent field calculations. *Journal of Computational Chemistry*, 39(15):909–916, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kandathil:2013:ATK

[KFY+13] Shaun M. Kandathil, Timothy L. Fletcher, Yongna Yuan, Joshua Knowles, and Paul L. A. Popelier. Accuracy and tractability of a kriging model of intramolecular polarizable multipolar electrostatics and its application to histidine. *Journal of Computational Chemistry*, 34(21):1850–1861, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kesharwani:2011:PSE

[KG11] Manoj K. Kesharwani and Bishwajit Ganguly. Probing the structural and electronic effects to stabilize nonplanar forms of thioamide derivatives: a computational study. *Journal of Computational Chemistry*, 32(10):2170–2176, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koukos:2013:SNU

[KG13] Panagiotis I. Koukos and Nicholas M. Glykos. Software news and updates: Grcarma: a fully automated task-oriented interface for the analysis of molecular dynamics trajectories. *Journal of Computational Chemistry*, 34(26):2310–2312, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karton:2015:ARB

[KG15] Amir Karton and Lars Goerigk. Accurate reaction barrier heights of pericyclic reactions: Surprisingly large deviations for the CBS-QB3 composite method and their consequences in DFT benchmark studies. *Journal of Computational Chemistry*, 36(9):622–632, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kazachenko:2015:AGB

[KGHC15] Sergey Kazachenko, Mark Giovinazzo, Kyle Wm. Hall, and Natalie M. Cann. Algorithms for GPU-based molecular dynamics simulations of complex fluids: Applications to water, mixtures, and liquid crystals. *Journal of Computational Chemistry*, 36(24):1787–1804, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaukonen:2012:LJP

[KGHK12] M. Kaukonen, A. Gulans, P. Havu, and E. Kauppinen. Lennard-Jones parameters for small diameter carbon nanotubes and water for molecular mechanics simulations from van der Waals density functional calculations. *Journal of*

Computational Chemistry, 33(6):652–658, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kong:2019:IDM

[KGJZ19] Chui-Peng Kong, Xin Gao, Ran Jia, and Hong-Xing Zhang. Investigating detailed mechanism of hydrogen molecules adsorbing on single-wall carbon nanotubes using fitted force field parameters containing carbon-carbon interactions. *Journal of Computational Chemistry*, 40(10):1073–1083, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kramer:2012:AME

[KGM12] Christian Kramer, Peter Gedeck, and Markus Meuwly. Atomic multipoles: Electrostatic potential fit, local reference axis systems, and conformational dependence. *Journal of Computational Chemistry*, 33(20):1673–1688, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaupp:2016:ETP

[KGR+16] Martin Kaupp, Simon Gückel, Manuel Renz, Sascha Klawohn, Kolja Theilacker, Matthias Parthey, and Christoph Lambert. Electron transfer pathways in mixed-valence paracyclophane-bridged bis-triarylamine radical cations. *Journal of Computational Chemistry*, 37(1):93–102, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kimura:2019:CSE

[KHE+19] Ryuto Kimura, Yuh Hijikata, Clothilde A. Eveleens, Alister J. Page, and Stephan Irle. Chiral-selective etching effects on carbon nanotube growth at edge carbon atoms. *Journal of Computational Chemistry*, 40(2):375–380, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaledin:2019:BAL

[KHLM19] Alexey L. Kaledin, Craig L. Hill, Tianquan Lian, and Djamaladdin G. Musaev. A bulk adjusted linear combination of atomic orbitals (BA-LCAO) approach for nanoparticles. *Journal of Computational Chemistry*, 40(1):212–221, January 5,

2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kearns:2017:CCF

[KHWB17] Fiona L. Kearns, Phillip S. Hudson, Henry L. Woodcock, and Stefan Boresch. Computing converged free energy differences between levels of theory via nonequilibrium work methods: Challenges and opportunities. *Journal of Computational Chemistry*, 38(16):1376–1388, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kido:2019:NMF

[Kid19] Kentaro Kido. A noniterative mean-field QM/MM-type approach with a linear response approximation toward an efficient free-energy evaluation. *Journal of Computational Chemistry*, 40(24):2072–2085, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kashimura:2019:PES

[KIOY19] Tatsuhiko Kashimura, Tomoya Ikezaki, Yusuke Ohta, and Satoshi Yabushita. Potential energy surfaces and nonadiabatic transitions in the asymptotic regions of ICN photodissociation to study the interference effects in the F_1 and F_2 spin-rotation levels of the CN products. *Journal of Computational Chemistry*, 40(2):482–499, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ko:2010:CIC

[KJ10] Youn Jo Ko and Won Ho Jo. Chloride ion conduction without water coordination in the pore of ClC protein. *Journal of Computational Chemistry*, 31(3):603–611, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kessler:2012:BEF

[KJDB12] Jiří Kessler, Milan Jakubek, Bohumil Dolenský, and Petr Bouř. Binding energies of five molecular pincers calculated by explicit and implicit solvent models. *Journal of Computational Chemistry*, 33(29):2310–2317, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kobayashi:2017:SNU

[KJM+17] Chigusa Kobayashi, Jaewoon Jung, Yasuhiro Matsunaga, Takaharu Mori, Tadashi Ando, Koichi Tamura, Motoshi Kamiya, and Yuji Sugita. Software news and updates: GENESIS 1.1: a hybrid-parallel molecular dynamics simulator with enhanced sampling algorithms on multiple computational platforms. *Journal of Computational Chemistry*, 38 (25):2193–2206, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaliman:2017:SNU

[KK17a] Ilya A. Kaliman and Anna I. Krylov. Software news and updates: New algorithm for tensor contractions on multi-core CPUs, GPUs, and accelerators enables CCSD and EOM-CCSD calculations with over 1000 basis functions on a single compute node. *Journal of Computational Chemistry*, 38(11): 842–853, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krause:2017:SNU

[KK17b] Katharina Krause and Wim Klopper. Software news and updates: Implementation of the Bethe–Salpeter equation in the TURBOMOLE program. *Journal of Computational Chemistry*, 38(6):383–388, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kroeger:2019:CFM

[KK19] Asja A. Kroeger and Amir Karton. A computational foray into the mechanism and catalysis of the adduct formation reaction of guanine with crotonaldehyde. *Journal of Computational Chemistry*, 40(4):630–637, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:2018:AER

[KKA+18] Yusuke Kondo, Masato Kobayashi, Tomoko Akama, Takeshi Noro, and Tetsuya Taketsugu. All-electron relativistic computations on the low-lying electronic states, bond length, and vibrational frequency of CeF diatomic molecule with spin-orbit coupling effects. *Journal of Computational Chemistry*, 39(16): 964–972, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kyriakidou:2019:DQP

[KKGW19] Katerina Kyriakidou, Padeleimon Karafiloglou, Eric Glendening, and Frank Weinhold. To be or not to be: Demystifying the 2nd-quantized picture of complex electronic configuration patterns in chemistry with natural poly-electron population analysis. *Journal of Computational Chemistry*, 40(15):1509–1520, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kuenzer:2018:PVC

[KKH18] Ulrich Kuenzer, Martin Klotz, and Thomas S. Hofer. Probing vibrational coupling via a grid-based quantum approach — an efficient strategy for accurate calculations of localized normal modes in solid-state systems. *Journal of Computational Chemistry*, 39(26):2196–2209, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaledin:2019:EST

[KKH19] Leonid A. Kaledin, Alexey L. Kaledin, and Michael C. Heaven. The electronic structure of thorium monoxide: Ligand field assignment of states in the range 0–5 eV. *Journal of Computational Chemistry*, 40(2):430–446, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:2019:HBD

[KKK+19] Hiroko X. Kondo, Ayumi Kusaka, Colin K. Kitakawa, Jinta Onari, Shusuke Yamanaka, Haruki Nakamura, and Yu Takano. Hydrogen bond donors and acceptors are generally depolarized in α-helices as revealed by a molecular tailoring approach. *Journal of Computational Chemistry*, 40(23): 2043–2052, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kornobis:2013:ESS

[KKL+13] Karina Kornobis, Neeraj Kumar, Piotr Lodowski, Maria Jaworska, Piotr Piecuch, Jesse J. Lutz, Bryan M. Wong, and Pawel M. Kozlowski. Electronic structure of the S_1 state in methylcobalamin: Insight from CASSCF/MC-XQDPT2, EOM-CCSD, and TD-DFT calculations. *Journal of Computational Chemistry*, 34(12):987–1004, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Katouda:2011:TLH

[KKNN11] Michio Katouda, Masato Kobayashi, Hiromi Nakai, and Shigeru Nagase. Two-level hierarchical parallelization of second-order Møller–Plesset perturbation calculations in divide-and-conquer method. *Journal of Computational Chemistry*, 32(13):2756–2764, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klimenko:2016:NEA

[KKO+16] Kyrylo Klimenko, Victor Kuz'min, Liudmila Ognichenko, Leonid Gorb, Manoj Shukla, Natalia Vinas, Edward Perkins, Pavel Polishchuk, Anatoly Artemenko, and Jerzy Leszczynski. Novel enhanced applications of QSPR models: Temperature dependence of aqueous solubility. *Journal of Computational Chemistry*, 37(22):2045–2051, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karagiannis:2011:DFS

[KKPT11] Efstathios E. Karagiannis, Christos E. Kefalidis, Ioanna Petrakopoulou, and Constantinos A. Tsipis. Density functional study of structural, electronic, and optical properties of small bimetallic ruthenium-copper clusters. *Journal of Computational Chemistry*, 32(7):1241–1261, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kerber:2013:SNU

[KKR+13] Torsten Kerber, Rachel Nathaniel Kerber, Xavier Rozanska, Philippe Sautet, and Paul Fleurat-Lessard. Software news and updates: QMX: a versatile environment for hybrid calculations applied to the grafting of $Al_2Cl_3Me_3$ on a silica surface. *Journal of Computational Chemistry*, 34(13):1155–1163, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kingsley:2014:ILI

[KL14] Laura J. Kingsley and Markus A. Lill. Including ligand-induced protein flexibility into protein tunnel prediction. *Journal of Computational Chemistry*, 35(24):1748–1756, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2017:SNU

[KLJ+17] Seonghoon Kim, Jumin Lee, Sunhwan Jo, Charles L. Brooks III, Hui Sun Lee, and Wonpil Im. Software news and updates: CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. *Journal of Computational Chemistry*, 38(21):1879–1886, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kendrick:2012:EVW

[KLN12] John Kendrick, Frank J. J. Leusen, and Marcus A. Neumann. Empirical van der Waals corrections to solid-state density functional theory: Iodine and phosphorous containing molecular crystals. *Journal of Computational Chemistry*, 33(19): 1615–1622, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kwon:2016:SCE

[KLN16] Junpyo Kwon, Myeongsang Lee, and Sungsoo Na. Sodium chloride's effect on self-assembly of diphenylalanine bilayer. *Journal of Computational Chemistry*, 37(19):1839–1846, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knapp:2010:VPR

[KLOS10] Bernhard Knapp, Nadja Lederer, Ulrich Omasits, and Wolfgang Schreiner. vmdICE: a plug-in for rapid evaluation of molecular dynamics simulations using VMD. *Journal of Computational Chemistry*, 31(16):2868–2873, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozlowska:2010:DSCa

[KLS10] Urszula Kozłowska, Adam Liwo, and Harold A. Scheraga. Determination of side-chain-rotamer and side-chain and backbone virtual-bond-stretching potentials of mean force from AM1 energy surfaces of terminally-blocked amino-acid residues, for coarse-grained simulations of protein structure and folding. I. The method. *Journal of Computational Chemistry*, 31(6):1143–1153, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khan:2018:HPT

[KLZ+18] Jahanzeb Khan, Yunpeng Liu, Tianqi Zhao, Hua Geng, Wei Xu, and Zhigang Shuai. High performance thermoelectric materials based on metal organic coordination polymers through first-principles band engineering. *Journal of Computational Chemistry*, 39(31):2582–2588, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozuch:2013:SCS

[KM13] Sebastian Kozuch and Jan M. L. Martin. Spin-component-scaled double hybrids: an extensive search for the best fifth-rung functionals blending DFT and perturbation theory. *Journal of Computational Chemistry*, 34(27):2327–2344, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozlowska:2010:DSCb

[KMLS10] Urszula Kozłowska, Gia G. Maisuradze, Adam Liwo, and Harold A. Scheraga. Determination of side-chain-rotamer and side-chain and backbone virtual-bond-stretching potentials of mean force from AM1 energy surfaces of terminally-blocked amino-acid residues, for coarse-grained simulations of protein structure and folding. II. Results, comparison with statistical potentials, and implementation in the UNRES force field. *Journal of Computational Chemistry*, 31(6):1154–1167, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kawakami:2019:DCC

[KMS+19] Takashi Kawakami, Koichi Miyagawa, Sandeep Sharma, Toru Saito, Mitsuo Shoji, Satoru Yamada, Shusuke Yamanaka, Mitsutaka Okumura, Takahito Nakajima, and Kizashi Yamaguchi. UNO DMRG CAS CI calculations of binuclear manganese complex $Mn(IV)_2O_2$ $(NHCHCO_2)_4$: Scope and applicability of Heisenberg model. *Journal of Computational Chemistry*, 40(2):333–341, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ketrat:2019:TSM

[KMT+19] Sombat Ketrat, Thana Maihom, Piti Treesukul, Bundet Boekfa, and Jumras Limtrakul. Theoretical study of methane adsorption and C-H bond activation over Fe-embedded graphene: Effect of external electric field. *Journal of Computational Chemistry*, 40(32):2819–2826, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Katouda:2017:MOH

[KN17] Michio Katouda and Takahito Nakajima. MPI/OpenMP hybrid parallel algorithm for resolution of identity second-order Møller–Plesset perturbation calculation of analytical energy gradient for massively parallel multicore supercomputers. *Journal of Computational Chemistry*, 38(8):489–507, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2011:DDB

[KNE11a] Jae In Kim, Sungsoo Na, and Kilho Eom. Domain decomposition-based structural condensation of large protein structures for understanding their conformational dynamics. *Journal of Computational Chemistry*, 32(1):161–169, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kneller:2011:CFD

[Kne11b] Gerald R. Kneller. Comment on "Fast determination of the optimal rotational matrix for macromolecular superpositions" [J. Comp. Chem. **31**, 1561 (2010)]. *Journal of Computational Chemistry*, 32(1):183–184, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [LAT10] and reply [LAT11].

Katouda:2016:MPA

[KNHN16] Michio Katouda, Akira Naruse, Yukihiko Hirano, and Takahito Nakajima. Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers. *Journal of Computational Chemistry*, 37(30):2623–2633, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kjaer:2012:NMR

[KNP$^+$12] Hanna Kjær, Monia R. Nielsen, Gabriel I. Pagola, Marta B. Ferraro, Paolo Lazzeretti, and Stephan P. A. Sauer. Nuclear magnetic resonance J coupling constant polarizabilities of hydrogen peroxide: a basis set and correlation study. *Journal* *of Computational Chemistry*, 33(23):1845–1853, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kramer:2018:ECO

[KNR+18] Tobias Kramer, Matthias Noack, Alexander Reinefeld, Mirta Rodríguez, and Yaroslav Zelinskyy. Efficient calculation of open quantum system dynamics and time-resolved spectroscopy with distributed memory HEOM (DM–HEOM). *Journal of Computational Chemistry*, 39(22):1779–1794, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karamanis:2014:SNO

[KOP+14] Panaghiotis Karamanis, Nicolás Otero, Claude Pouchan, Juan José Torres, William Tiznado, Aggelos Avramopoulos, and Manthos G. Papadopoulos. Significant nonlinear-optical switching capacity in atomic clusters built from silicon and lithium: a combined ab initio and density functional study. *Journal of Computational Chemistry*, 35(11):829–838, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2015:IGS

[Kop15a] Jacek Koput. Ab initio ground-state potential energy function and vibration-rotation energy levels of imidogen, NH. *Journal of Computational Chemistry*, 36(17):1286–1294, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2015:ISC

[Kop15b] Jacek Koput. Ab initio spectroscopic characterization of borane, BH, in its X $^1\Sigma^+$ electronic state. *Journal of Computational Chemistry*, 36(30):2219–2227, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2016:IPE

[Kop16] Jacek Koput. Ab initio potential energy surface and vibration-rotation energy levels of silicon dicarbide, SiC_2. *Journal of Computational Chemistry*, 37(26):2395–2402, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2017:IPEa

[Kop17a] Jacek Koput. Ab initio potential energy surface and vibration-rotation energy levels of beryllium monohydroxide. *Journal of Computational Chemistry*, 38(1):37–43, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2017:IPEb

[Kop17b] Jacek Koput. Ab initio potential energy surface and vibration-rotation energy levels of sulfur dioxide. *Journal of Computational Chemistry*, 38(12):892–900, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2018:IPE

[Kop18] Jacek Koput. Ab initio potential energy surface and vibration-rotation energy levels of germanium dicarbide, GeC_2. *Journal of Computational Chemistry*, 39(19):1327–1334, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2019:IGS

[Kop19a] Jacek Koput. Ab initio ground-state potential energy function and vibration–rotation energy levels of aluminum monohydride. *Journal of Computational Chemistry*, 40(29):2522–2529, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2019:ISV

[Kop19b] Jacek Koput. Ab initio structure and vibration-rotation dynamics of germylene, GeH_2. *Journal of Computational Chemistry*, 40(21):1911–1918, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kosenkov:2016:SNU

[Kos16] Dmytro Kosenkov. Software news and updates: PyFREC: Software for Förster electronic coupling evaluation in molecular fragments. *Journal of Computational Chemistry*, 37(19): 1847–1854, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kowal:2011:IMG

[Kow11] Andrzej T. Kowal. Ab initio molecular geometry and anharmonic vibrational spectra of thiourea and thiourea-d_4. *Journal of Computational Chemistry*, 32(4):718–729, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2012:SHM

[KOY+12] Tae-Rae Kim, Sangho Oh, Joshua SungWoo Yang, Sanghyuk Lee, Seokmin Shin, and Jinhyuk Lee. A simplified homology-model builder toward highly protein-like structures: an inspection of restraining potentials. *Journal of Computational Chemistry*, 33(24):1927–1935, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2010:IEC

[KP10] K. Senthil Kumar and Archita Patnaik. Intramolecular electronic communication in a dimethylaminoazobenzene–fullerene C_{60} dyad: an experimental and TD-DFT study. *Journal of Computational Chemistry*, 31(6):1182–1194, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozlowski:2011:NIQ

[KP11] David Kozlowski and Julien Pilmé. New insights in quantum chemical topology studies using numerical grid-based analyses. *Journal of Computational Chemistry*, 32(15):3207–3217, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kutzner:2015:SNU

[KPF+15] Carsten Kutzner, Szilárd Páll, Martin Fechner, Ansgar Esztermann, Bert L. de Groot, and Helmut Grubmüller. Software news and updates: Best bang for your buck: GPU nodes for GROMACS biomolecular simulations. *Journal of Computational Chemistry*, 36(26):1990–2008, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kutzner:2019:MBY

[KPF+19] Carsten Kutzner, Szilárd Páll, Martin Fechner, Ansgar Esztermann, Bert L. de Groot, and Helmut Grubmüller. More bang for your buck: Improved use of GPU nodes for GROMACS 2018. *Journal of Computational Chemistry*, 40(27): 2418–2431, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kozlov:2018:CES

[KPG18] Maxim I. Kozlov, Vladimir V. Poddubnyy, and Ilya O. Glebov. Calculation of the excited states properties of LH1 complex of *Thermochromatium tepidum*. *Journal of Computational Chemistry*, 39(21):1599–1606, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khanh:2019:ICB

[KPH+19] Pham N. Khanh, Cam-Tu D. Phan, Dai Q. Ho, Quan Van Vo, Vu T. Ngan, Minh Tho Nguyen, and Nguyen T. Trung. Insights into the cooperativity between multiple interactions of dimethyl sulfoxide with carbon dioxide and water. *Journal of Computational Chemistry*, 40(2):464–474, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2013:PEO

[KPL13] Hyungjun Kim, Joungwon Park, and Yoon Sup Lee. A protocol to evaluate one electron redox potential for iron complexes. *Journal of Computational Chemistry*, 34(26):2233–2241, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2015:PRP

[KPL15] Hyungjun Kim, Joungwon Park, and Yoon Sup Lee. Prediction of the reduction potential of tris(2,2′-bipyridinyl)iron(III/II) derivatives. *Journal of Computational Chemistry*, 36(1): 33–41, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2012:MSD

[KR12] Hyun Woo Kim and Young Min Rhee. Molecule-specific determination of atomic polarizabilities with the polarizable atomic multipole model. *Journal of Computational Chemistry*, 33 (20):1662–1672, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karbowiak:2014:LES

[KR14] Mirosław Karbowiak and Czesław Rudowicz. Letters to the Editor: Software package SIMPRE — revisited. *Journal of Computational Chemistry*, 35(26):1935–1941, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krissinel:2010:CCN

[Kri10] Evgeny Krissinel. Crystal contacts as nature's docking solutions. *Journal of Computational Chemistry*, 31(1):133–143, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2012:BDV

[KRSC12] Deok-Soo Kim, Joonghyun Ryu, Hayong Shin, and Youngsong Cho. Beta-decomposition for the volume and area of the union of three-dimensional balls and their offsets. *Journal of Computational Chemistry*, 33(13):1252–1273, May 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaminsky:2010:CBS

[KRTB10] Jakub Kaminský, Ivan Raich, Kateřina Tomčáková, and Petr Bouř. Conformational behavior of simple furanosides studied by optical rotation. *Journal of Computational Chemistry*, 31 (11):2213–2224, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koppole:2012:DRP

[KS12] Sampath Koppole and Michael Schaefer. A discriminative Ramachandran potential of mean force aimed at minimizing secondary structure bias. *Journal of Computational Chemistry*, 33(7):791–799, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaliman:2013:SNU

[KS13a] Ilya A. Kaliman and Lyudmila V. Slipchenko. Software news and updates: LIBEFP: a new parallel implementation of the effective fragment potential method as a portable software library. *Journal of Computational Chemistry*, 34(26):2284–2292, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kovacevic:2013:TSM

[KS13b] Goran Kovacevic and Aleksandar Sabljic. Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene. *Journal of Computational Chemistry*, 34(8): 646–655, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaliman:2015:SNU

[KS15] Ilya A. Kaliman and Lyudmila V. Slipchenko. Software news and updates: Hybrid MPI/OpenMP parallelization of the effective fragment potential method in the `libefp` software library. *Journal of Computational Chemistry*, 36(2):129–135, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kasahara:2018:TDP

[KS18] Kento Kasahara and Hirofumi Sato. Time-dependent pair distribution functions based on Smoluchowski equation and application to an electrolyte solution. *Journal of Computational Chemistry*, 39(20):1491–1497, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kulsha:2019:SS

[KS19] Andrey V. Kulsha and Dmitry I. Sharapa. Superhalogen and superacid. *Journal of Computational Chemistry*, 40(26):2293–2300, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kraka:2016:REB

[KSC16] Elfi Kraka, Dani Setiawan, and Dieter Cremer. Re-evaluation of the bond length–bond strength rule: the stronger bond is not always the shorter bond. *Journal of Computational Chemistry*, 37(1):130–142, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kulp:2012:SIM

[KSD+12] Daniel W. Kulp, Sabareesh Subramaniam, Jason E. Donald, Brett T. Hannigan, Benjamin K. Mueller, Gevorg Grigoryan, and Alessandro Senes. Structural informatics, modeling, and design with an open-source Molecular Software Library (MSL). *Journal of Computational Chemistry*, 33(20):1645–

1661, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kar:2013:LRCa

[KSH13] Rahul Kar, Jong-Won Song, and Kimihiko Hirao. Long-range corrected functionals satisfy Koopmans' theorem: Calculation of correlation and relaxation energies. *Journal of Computational Chemistry*, 34(11):958–964, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krupicka:2017:TAG

[KSH+17] Martin Krupička, Kantharuban Sivalingam, Lee Huntington, Alexander A. Auer, and Frank Neese. A toolchain for the automatic generation of computer codes for correlated wavefunction calculations. *Journal of Computational Chemistry*, 38(21):1853–1868, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kollmar:2019:PBS

[KSHP+19] Christian Kollmar, Kantharuban Sivalingam, Benjamin Helmich-Paris, Celestino Angeli, and Frank Neese. A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. *Journal of Computational Chemistry*, 40(14):1463–1470, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kjaer:2011:CCP

[KSK11] Hanna Kjær, Stephan P. A. Sauer, and Jacob Kongsted. The coupling constant polarizability and hyperpolarizabilty of ^{1}J (NH) in *N*-methylacetamide, and its application for the multipole spin–spin coupling constant polarizability/reaction field approach to solvation. *Journal of Computational Chemistry*, 32(15):3168–3174, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karton:2016:HFP

[KSM16] Amir Karton, Peter R. Schreiner, and Jan M. L. Martin. Heats of formation of platonic hydrocarbon cages by means of high-level thermochemical procedures. *Journal of Computational Chemistry*, 37(1):49–58, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karton:2017:WDH

[KSM17] Amir Karton, Nitai Sylvetsky, and Jan M. L. Martin. W4-17: a diverse and high-confidence dataset of atomization energies for benchmarking high-level electronic structure methods. *Journal of Computational Chemistry*, 38(24):2063–2075, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kawashima:2019:PIM

[KSNT19] Yukio Kawashima, Keisuke Sawada, Takahito Nakajima, and Masanori Tachikawa. A path integral molecular dynamics study on intermolecular hydrogen bond of acetic acid-arsenic acid anion and acetic acid-phosphoric acid anion clusters. *Journal of Computational Chemistry*, 40(1):172–180, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kawashima:2019:TIR

[KSO+19] Kyohei Kawashima, Takehiro Sato, Masamichi Ogasawara, Ken Kamikawa, and Seiji Mori. Theoretical investigations of Rh-catalyzed asymmetric 1,4-addition to enones using planar-chiral phosphine-olefin ligands. *Journal of Computational Chemistry*, 40(1):113–118, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koster:2016:AAI

[KSR+16] Andreas Köster, Thomas Spura, Gábor Rutkai, Jan Kessler, Hendrik Wiebeler, Jadran Vrabec, and Thomas D. Kühne. Assessing the accuracy of improved force-matched water models derived from ab initio molecular dynamics simulations. *Journal of Computational Chemistry*, 37(19):1828–1838, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krausbeck:2017:SAF

[KSR17] Florian Krausbeck, Jan-Grimo Sobez, and Markus Reiher. Stabilization of activated fragments by shell-wise construction of an embedding environment. *Journal of Computational Chemistry*, 38(14):1023–1038, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kar:2013:LRCb

[KSSH13] Rahul Kar, Jong-Won Song, Takeshi Sato, and Kimihiko Hirao. Long-range corrected density functionals combined with local response dispersion: a promising method for weak interactions. *Journal of Computational Chemistry*, 34(27):2353–2359, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kuttel:2016:SNU

[KSW16] Michelle M. Kuttel, Jonas Ståhle, and Göran Widmalm. Software news and updates: CarbBuilder: Software for building molecular models of complex oligo- and polysaccharide structures. *Journal of Computational Chemistry*, 37(22):2098–2105, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kleesiek:2010:RSS

[KT10] Jens Kleesiek and Andrew E. Torda. RNA secondary structure prediction using a self-consistent mean field approach. *Journal of Computational Chemistry*, 31(6):1135–1142, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kefalidis:2012:DSM

[KT12] Christos E. Kefalidis and Constantinos A. Tsipis. DFT study of the mechanism of hydroamination of ethylene with ammonia catalyzed by diplatinum(II) complexes: Inner- or outer-sphere? *Journal of Computational Chemistry*, 33(20):1689–1700, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kowsari:2018:SER

[KT18] Mohammad H. Kowsari and Leila Tohidifar. Systematic evaluation and refinement of existing all-atom force fields for the simulation of liquid acetonitrile. *Journal of Computational Chemistry*, 39(23):1843–1853, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kamiya:2019:ISH

[KT19] Muneaki Kamiya and Tetsuya Taketsugu. Ab initio surface hopping excited-state molecular dynamics approach on the basis of spin-orbit coupled states: an application to the A-band photodissociation of CH_3I. *Journal of Computational Chemistry*, 40(2):456–463, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirkpatrick:2017:ECI

[KTK17] Charles C. Kirkpatrick, John N. Truong, and Bruce A. Kowert. *d*-electron count, ion-pairing and diagonal twist angles in metallo-bis(dithiolene) complexes. *Journal of Computational Chemistry*, 38(2):93–100, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koyano:2010:OSS

[KTNN10] Yoshiyuki Koyano, Norio Takenaka, Yukinori Nakagawa, and Masataka Nagaoka. An optimum strategy for solution chemistry using semiempirical molecular orbital method. II. Primary importance of reproducing electrostatic interaction in the QM/MM framework. *Journal of Computational Chemistry*, 31(14):2628–2641, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kokubo:2011:IPP

[KTO11] Hironori Kokubo, Toshimasa Tanaka, and Yuko Okamoto. Ab initio prediction of protein–ligand binding structures by replica-exchange umbrella sampling simulations. *Journal of Computational Chemistry*, 32(13):2810–2821, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kokubo:2013:TDR

[KTO13] Hironori Kokubo, Toshimasa Tanaka, and Yuko Okamoto. Two-dimensional replica-exchange method for predicting protein–ligand binding structures. *Journal of Computational Chemistry*, 34(30):2601–2614, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klenin:2011:DMS

[KTSW11] Konstantin V. Klenin, Frank Tristram, Timo Strunk, and Wolfgang Wenzel. Derivatives of molecular surface area and volume: Simple and exact analytical formulas. *Journal of Computational Chemistry*, 32(12):2647–2653, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kanematsu:2016:IUE

[KTT16] Yusuke Kanematsu, Masanori Tachikawa, and Yu Takano. Inverse Ubbelohde effect in the short hydrogen bond of photosystem II: Relation between H/D isotope effect and symmetry in potential energy profile. *Journal of Computational Chemistry*, 37(23):2140–2145, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kashmirian:2012:MDE

[KUDG12] Jennifer M. Kashmirian, Alfred Uhlherr, Alan Dorin, and David G. Green. Molecular dynamics extended for fluctuating networks: Application to water. *Journal of Computational Chemistry*, 33(15):1364–1373, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kadam:2012:NAM

[KV12] Shantanu Kadam and Kumar Vanka. A new approximate method for the stochastic simulation of chemical systems: the representative reaction approach. *Journal of Computational Chemistry*, 33(3):276–285, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kadam:2013:SPN

[KV13] Shantanu Kadam and Kumar Vanka. Solving the problem of negative populations in approximate accelerated stochastic simulations using the representative reaction approach. *Journal of Computational Chemistry*, 34(5):394–404, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaur:2014:MIN

[KV14] Gurpreet Kaur and Vikas. On the mechanism of intramolecular nitrogen-atom hopping in the carbon chain of C_6N radical: a plausible 3c–4e crossover π–long-bond. *Journal of Computational Chemistry*, 35(21):1568–1576, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krieger:2015:NWB

[KV15a] Elmar Krieger and Gert Vriend. New ways to boost molecular dynamics simulations. *Journal of Computational Chemistry*, 36(13):996–1007, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kuriakose:2015:CSA

[KV15b] Nishamol Kuriakose and Kumar Vanka. Can substituted allenes be highly efficient leaving groups in catalytic processes? A computational investigation. *Journal of Computational Chemistry*, 36(11):795–804, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karolak:2014:ESS

[KvdV14] Aleksandra Karolak and Arjan van der Vaart. Enhanced sampling simulations of DNA step parameters. *Journal of Computational Chemistry*, 35(32):2297–2304, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karimi-Varzaneh:2011:IMD

[KVQC+11] Hossein Ali Karimi-Varzaneh, Hu-Jun Qian, Xiaoyu Chen, Paola Carbone, and Florian Müller-Plathe. IBIsCO: a molecular dynamics simulation package for coarse-grained simulation. *Journal of Computational Chemistry*, 32(7):1475–1487, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kritayakornupong:2010:IQM

[KVR10] Chinapong Kritayakornupong, Viwat Vchirawongkwin, and Bernd M. Rode. An ab initio quantum mechanical charge field molecular dynamics simulation of a dilute aqueous HCl solution. *Journal of Computational Chemistry*, 31(8):1785–1792, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kubar:2015:SNU

[KWG15] Tomáš Kubař, Kai Welke, and Gerrit Groenhof. Software news and updates: New QM/MM implementation of the DFTB3 method in the `gromacs` package. *Journal of Computational Chemistry*, 36(26):1978–1989, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kratz:2016:SNU

[KWL+16] Eric G. Kratz, Alice R. Walker, Louis Lagardère, Filippo Lipparini, Jean-Philip Piquemal, and G. Andrés Cisneros. Software news and updates: LICHEM: a QM/MM program for simulations with multipolar and polarizable force fields. *Journal of Computational Chemistry*, 37(11):1019–1029, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Knight:2013:AQA

[KYB13] Jennifer L. Knight, Joseph D. Yesselman, and Charles L. Brooks III. Assessing the quality of absolute hydration free energies among CHARMM-compatible ligand parameterization schemes. *Journal of Computational Chemistry*, 34(11): 893–903, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2011:ECE

[KYCL11] Jongtaek Kim, Eunjung Yoo, Sukbok Chang, and Yoon Sup Lee. Electronic and chelation effects on the unusual C2-methylation of *N*-(para-substituted)phenylaziridines with lithium organocuprates. *Journal of Computational Chemistry*, 32(9):1859–1868, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2015:SNU

[KYG+15] Anmol Kumar, Sachin D. Yeole, Shridhar R. Gadre, Rafael López, Jaime F. Rico, Guillermo Ramírez, Ignacio Ema, and David Zorrilla. Software news and updates: DAMQT 2.1.0: a new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. *Journal of Computational Chemistry*, 36 (31):2350–2359, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirilchuk:2015:MPF

[KYKR15] Andrey A. Kirilchuk, Aleksandr A. Yurchenko, Aleksandr N. Kostyuk, and Alexander B. Rozhenko. 1,2-migration in *N*-phosphano functionalized *N*-heterocyclic carbenes. *Journal of Computational Chemistry*, 36(1):42–48, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kajiwara:2017:ITM

[KYT+17] Yuta Kajiwara, Satoshi Yasuda, Yuuki Takamuku, Takeshi Murata, and Masahiro Kinoshita. Identification of thermostabilizing mutations for a membrane protein whose three-dimensional structure is unknown. *Journal of Computational Chemistry*, 38(4):211–223, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koukaras:2012:SSE

[KZK+12] Emmanuel N. Koukaras, Aristides D. Zdetsis, Panaghiotis Karamanis, Claude Pouchan, Aggelos Avramopoulos, and Manthos G. Papadopoulos. Structural and static electric response properties of highly symmetric lithiated silicon cages: Theoretical predictions. *Journal of Computational Chemistry*, 33(10):1068–1079, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krajniak:2018:CGM

[KZP+18a] Jakub Krajniak, Zidan Zhang, Sudharsan Pandiyan, Eric Nies, and Giovanni Samaey. Coarse-grained molecular dynamics simulations of polymerization with forward and backward reactions. *Journal of Computational Chemistry*, 39(22): 1764–1778, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krajniak:2018:RMM

[KZP+18b] Jakub Krajniak, Zidan Zhang, Sudharsan Pandiyan, Eric Nies, and Giovanni Samaey. Reverse mapping method for complex polymer systems. *Journal of Computational Chemistry*, 39(11):648–664, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Keceli:2016:SIP

[KZZ+16] Murat Keçeli, Hong Zhang, Peter Zapol, David A. Dixon, and Albert F. Wagner. Shift-and-invert parallel spectral transformation eigensolver: Massively parallel performance for density-functional based tight-binding. *Journal of Computational Chemistry*, 37(4):448–459, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Labonte:2017:RCM

[LABSG17] Jason W. Labonte, Jared Adolf-Bryfogle, William R. Schief, and Jeffrey J. Gray. Residue-centric modeling and design of saccharide and glycoconjugate structures. *Journal of Computational Chemistry*, 38(5):276–287, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lii:2016:CMM

[LAHS16] Jenn-Huei Lii, Norman L. Allinger, Ching-Han Hu, and Henry F. Schaefer III. Catenanes: a molecular mechanics analysis of the $(C_{13}H_{26})_2$ structure 13-13 D2. *Journal of Computational Chemistry*, 37(1):124–129, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lenchuk:2019:CSD

[LAM19] Olena Lenchuk, Philipp Adelhelm, and Doreen Mollenhauer. Comparative study of density functionals for the description of lithium-graphite intercalation compounds. *Journal of Computational Chemistry*, 40(27):2400–2412, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larin:2011:PAM

[Lar11] Alexander V. Larin. Point atomic multipole moments for simulation of electrostatic potential and field in all-siliceous zeolites. *Journal of Computational Chemistry*, 32(11):2459–2473, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laref:2012:TBM

[Lar12] A. Laref. Tight-binding molecular dynamics simulation of ZnSe liquid within the local environment dependence. *Journal of Computational Chemistry*, 33(1):1–10, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lundborg:2014:SNU

[LAS+14] Magnus Lundborg, Rossen Apostolov, Daniel Spångberg, Anders Gärdenäs, David van der Spoel, and Erik Lindahl. Software news and updates: An efficient and extensible format, library, and API for binary trajectory data from molecular simulations. *Journal of Computational Chemistry*, 35(3):260–269, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2010:FDO

[LAT10] Pu Liu, Dimitris K. Agrafiotis, and Douglas L. Theobald. Fast determination of the optimal rotational matrix for macromolecular superpositions. *Journal of Computational Chemistry*, 31(7):1561–1563, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [Kne11b] and reply [LAT11].

Liu:2011:RCR

[LAT11] Pu Liu, Dimitris K. Agrafiotis, and Douglas L. Theobald. Rapid communication reply to comment on: "Fast determination of the optimal rotational matrix for macromolecular superpositions". *Journal of Computational Chemistry*, 32(1): 185–186, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [LAT10, Kne11b].

Lv:2016:CEH

[LAW+16] Chao Lv, Erick W. Aitchison, Dongsheng Wu, Lianqing Zheng, Xiaolin Cheng, and Wei Yang. Comparative exploration of hydrogen sulfide and water transmembrane free energy surfaces via orthogonal space tempering free energy sampling. *Journal of Computational Chemistry*, 37(6):567–574, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Licari:2015:SNU

[LBB+15] Daniele Licari, Alberto Baiardi, Małgorzata Biczysko, Franco Egidi, Camille Latouche, and Vincenzo Barone. Software news and updates: Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMS-Draw tool. *Journal of Computational Chemistry*, 36(5):321–334, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laflamme:2012:SIS

[LBC+12] Patrick Laflamme, Alexandre Beaudoin, Thomas Chapaton, Claude Spino, and Armand Soldera. Simulated infrared spectra of triflic acid during proton dissociation. *Journal of Computational Chemistry*, 33(12):1190–1196, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lamine:2019:CCZ

[LBC+19] Walid Lamine, Salima Boughdiri, Lorraine Christ, Christophe Morell, and Henry Chermette. Coordination chemistry of Zn^{2+} with Sal(ph)en ligands: Tetrahedral coordination or penta-coordination? A DFT analysis. *Journal of Computational Chemistry*, 40(5):717–725, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lucas:2012:MDS

[LBDP12] Timothy R. Lucas, Brad A. Bauer, Joseph E. Davis, and Sandeep Patel. Molecular dynamics simulation of hydrated DPPC monolayers using charge equilibration force fields. *Journal of Computational Chemistry*, 33(2):141–152, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lazarski:2016:DFT

[ŁBGS16] Roman Łazarski, Asbjörn Manfred Burow, Lukáš Grajciar, and Marek Sierka. Density functional theory for molecular and periodic systems using density fitting and continuous fast multipole method: Analytical gradients. *Journal of Computational Chemistry*, 37(28):2518–2526, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laury:2011:HVF

[LBH+11] Marie L. Laury, Scott E. Boesch, Ian Haken, Pankaj Sinha, Ralph A. Wheeler, and Angela K. Wilson. Harmonic vibrational frequencies: Scale factors for pure, hybrid, hybrid meta, and double-hybrid functionals in conjunction with correlation consistent basis sets. *Journal of Computational Chemistry*, 32(11):2339–2347, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopes:2010:CDP

[LBS10] Anne Lopes, Marcel Schmidt Am Busch, and Thomas Simonson. Computational design of protein–ligand binding: Modifying the specificity of asparaginyl-tRNA synthetase. *Journal of Computational Chemistry*, 31(6):1273–1286, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lingam:2011:SEB

[LBTV11] Ch. Bheema Lingam, K. Ramesh Babu, Surya P. Tewari, and G. Vaitheeswaran. Structural, electronic, bonding, and elastic properties of NH_3BH_3: a density functional study. *Journal of Computational Chemistry*, 32(8):1734–1742, June 2011.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lingam:2012:DFS

[LBTV12] Ch. Bheema Lingam, K. Ramesh Babu, Surya P. Tewari, and G. Vaitheeswaran. Density functional study of electronic,bonding, and vibrational properties of $Ca(NH_2BH_3\ )_2$. *Journal of Computational Chemistry*, 33(9):987–997, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lai:2010:CSC

[LC10] Chin-Hung Lai and Pi-Tai Chou. A computational study on the capability of borane-cyclic boryl anion adducts to act as hydrogen atom donors. *Journal of Computational Chemistry*, 31(12):2258–2262, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2012:SNU

[LC12] Tian Lu and Feiwu Chen. Software news and updates: Multiwfn: a multifunctional wavefunction analyzer. *Journal of Computational Chemistry*, 33(5):580–592, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2016:MES

[LC16] Kuo Hao Lee and Jianhan Chen. Multiscale enhanced sampling of intrinsically disordered protein conformations. *Journal of Computational Chemistry*, 37(6):550–557, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2017:EIS

[LC17a] Kuo Hao Lee and Jianhan Chen. Efficacy of independence sampling in replica exchange simulations of ordered and disordered proteins. *Journal of Computational Chemistry*, 38(30): 2632–2640, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2017:OGI

[LC17b] Kuo Hao Lee and Jianhan Chen. Optimization of the GBMV2 implicit solvent force field for accurate simulation of protein conformational equilibria. *Journal of Computational Chemistry*, 38(16):1332–1341, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2017:DTE

[LCA17] Lin Li, Arghya Chakravorty, and Emil Alexov. DelPhiForce, a tool for electrostatic force calculations: Applications to macromolecular binding. *Journal of Computational Chemistry*, 38(9):584–593, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2010:RIC

[LCB10] Haiying Liu, Xiaohua Chen, and Yuxiang Bu. Redox-induced configuration conversion for thioacetamide dimer can function as a molecular switch. *Journal of Computational Chemistry*, 31(14):2533–2539, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2018:FAS

[LCC18] Yang Li, Junsheng Chen, and Tian-Shu Chu. Fluoride anion sensing mechanism of a BODIPY-linked hydrogen-bonding probe. *Journal of Computational Chemistry*, 39(21):1639–1647, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:NBO

[LCH10] Bin Li, Tian-Shu Chu, and Ke-Li Han. Non-Born–Oppenheimer dynamics calculations using the coherent switching with decay of mixing method. *Journal of Computational Chemistry*, 31(2):362–370, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2015:VWE

[LCH+15] Haisheng Li, Weiguang Chen, Xiaoyu Han, Liben Li, Qiang Sun, Zhengxiao Guo, and Yu Jia. Van der Waals effects on semiconductor clusters. *Journal of Computational Chemistry*, 36(25):1919–1927, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2018:MHT

[LCK+18] Wenlan Liu, Sofia Canola, Andreas Köhn, Bernd Engels, Fabrizia Negri, and Reinhold F. Fink. A model Hamiltonian tuned toward high level ab initio calculations to describe the character of excitonic states in perylenebisimide aggregates. *Journal of Computational Chemistry*, 39(24):1979–1989, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:TSH

[LCL+10] Wen-Zuo Li, Jian-Bo Cheng, Qing-Zhong Li, Bao-An Gong, and Jia-Zhong Sun. Theoretical study on HBO^+ and HOB^+ cations using multiconfiguration second-order perturbation theory. *Journal of Computational Chemistry*, 31(7):1397–1401, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2018:PFF

[LCL+18] Jian-Biao Liu, Xin Chen, Jun-Bo Lu, Hong-Qiang Cui, and Jun Li. Polarizable force field parameterization and theoretical simulations of $ThCl_4$ -LiCl molten salts. *Journal of Computational Chemistry*, 39(29):2432–2438, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lorenz:2014:BDG

[LCM+14] Marco Lorenz, Bartolomeo Civalleri, Lorenzo Maschio, Mauro Sgroi, and Daniele Pullini. Benchmarking dispersion and geometrical counterpoise corrections for cost-effective large-scale DFT calculations of water adsorption on graphene. *Journal of Computational Chemistry*, 35(24):1789–1800, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2016:DTI

[LCM16] Pingying Liu, Qiufeng Chen, and Jing Ma. Design of [2]rotaxane through image threshold segmentation of electrostatic potential image. *Journal of Computational Chemistry*, 37(24): 2228–2241, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2013:NBO

[LCPS13] Louis P. Lee, Daniel J. Cole, Mike C. Payne, and Chris-Kriton Skylaris. Natural bond orbital analysis in the ONETEP code: Applications to large protein systems. *Journal of Computa-*

tional Chemistry, 34(6):429–444, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laury:2012:VFS

[LCW12] Marie L. Laury, Matthew J. Carlson, and Angela K. Wilson. Vibrational frequency scale factors for density functional theory and the polarization consistent basis sets. *Journal of Computational Chemistry*, 33(30):2380–2387, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2010:FPS

[LCWW10] Qi Liang Lu, Li Li Chen, Jian Guo Wan, and Guang Hou Wang. First principles studies on the interaction of O_2 with $X@Al_{12}$ ($X = Al^-$, P^+, C, Si) clusters. *Journal of Computational Chemistry*, 31(15):2804–2809, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lizana:2018:TII

[LD18] Ignacio Lizana and Eduardo J. Delgado. Theoretical insights on the inhibition mechanism of a class A serine hydrolase by avibactam. *Journal of Computational Chemistry*, 39(24): 1943–1948, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lesch:2017:SNU

[LDB+17] Volker Lesch, Diddo Diddens, Carlos E. S. Bernardes, Benjamin Golub, Alain Dequidt, Veronika Zeindlhofer, Marcello Sega, and Christian Schröder. Software news and updates: ForConX: a forcefield conversion tool based on XML. *Journal of Computational Chemistry*, 38(9):629–638, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2015:APE

[LDG+15] Fang Liu, Likai Du, Jun Gao, Lili Wang, Bo Song, and Chengbu Liu. Application of polarizable ellipsoidal force field model to pnicogen bonds. *Journal of Computational Chemistry*, 36(7):441–448, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lyons:2014:PBC

[LDH+14] James Lyons, Abdollah Dehzangi, Rhys Heffernan, Alok Sharma, Kuldip Paliwal, Abdul Sattar, Yaoqi Zhou, and Yuedong Yang. Predicting backbone Cα angles and dihedrals from protein sequences by stacked sparse auto-encoder deep neural network. *Journal of Computational Chemistry*, 35(28): 2040–2046, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:NUH

[LDJ+10] Qing-Zhong Li, Xu Dong, Bo Jing, Wen-Zuo Li, Jian-Bo Cheng, Bao-An Gong, and Zhi-Wu Yu. A new unconventional halogen bond C — X$\cdots$H — M between HCCX (X = Cl and Br) and HMH (M = Be and Mg): an ab initio study. *Journal of Computational Chemistry*, 31(8):1662–1669, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2016:SFC

[LdSRR16] Jingbai Li, Giovana da Silva Ramos, and Andrey Yu Rogachev. Stability of functionalized corannulene cations [R-$C_{20}H_{10}$]$^+$: an influence of the nature of R-Group. *Journal of Computational Chemistry*, 37(25):2266–2278, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liang:2017:PRP

[LDZW17] Guangchao Liang, Nathan J. DeYonker, Xuan Zhao, and Charles Edwin Webster. Prediction of the reduction potential in transition-metal containing complexes: How expensive? For what accuracy? *Journal of Computational Chemistry*, 38 (28):2430–2438, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lage-Estebanez:2017:RER

[LEdOLdlV17] Isabel Lage-Estebanez, Lourdes del Olmo, Rafael López, and José Manuel García de la Vega. The role of errors related to DFT methods in calculations involving ion pairs of ionic liquids. *Journal of Computational Chemistry*, 38(8):530–540, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lehtola:2015:SNU

[Leh15] Susi Lehtola. Software news and updates: Automatic algorithms for completeness-optimization of Gaussian basis sets. *Journal of Computational Chemistry*, 36(5):335–347, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lesiuk:2019:ESV

[Les19] Michal Lesiuk. Efficient singular-value decomposition of the coupled-cluster triple excitation amplitudes. *Journal of Computational Chemistry*, 40(12):1319–1332, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Law:2014:PFE

[LFB14] Sean M. Law, Aaron T. Frank, and Charles L. Brooks III. PCASSO: a fast and efficient Cα-based method for accurately assigning protein secondary structure elements. *Journal of Computational Chemistry*, 35(24):1757–1761, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:QMR

[LFM12] Xue Li, Zheng Fu, and Kenneth M. Merz Jr. QM/MM refinement and analysis of protein bound retinoic acid. *Journal of Computational Chemistry*, 33(3):301–310, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:EGC

[LFN+10] Hui Li, Dmitri G. Fedorov, Takeshi Nagata, Kazuo Kitaura, Jan H. Jensen, and Mark S. Gordon. Energy gradients in combined fragment molecular orbital and polarizable continuum model (FMO/PCM) calculation. *Journal of Computational Chemistry*, 31(4):778–790, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ling:2011:STC

[LG11] Sanliang Ling and Maciej Gutowski. SSC: a tool for constructing libraries for systematic screening of conformers. *Journal of Computational Chemistry*, 32(9):2047–2054, July 15, 2011.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lucas:2014:UCM

[LG14] Xavier Lucas and Stefan Günther. Using chiral molecules as an approach to address low-druggability recognition sites. *Journal of Computational Chemistry*, 35(29):2114–2121, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2019:CIE

[LGC19] Yuanyuan Li, Yanzhen Gan, and Zexing Cao. Computational insight into excited states of the ring-opening radicals from the pyrolysis of furan biofuels. *Journal of Computational Chemistry*, 40(9):1057–1065, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lucke:2017:EPB

[LGKS17] Andreas Lücke, Uwe Gerstmann, Thomas D. Kühne, and Wolf G. Schmidt. Efficient PAW-based bond strength analysis for understanding the In/Si(111)(8×2)–(4×1) phase transition. *Journal of Computational Chemistry*, 38(26):2276–2282, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2011:CSS

[LGL11] Zhixiong Lin, Wilfred F. Van Gunsteren, and Haiyan Liu. Conformational state-specific free energy differences by one-step perturbation: Protein secondary structure preferences of the GROMOS 43A1 and 53A6 force fields. *Journal of Computational Chemistry*, 32(10):2290–2297, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lamsabhi:2015:EIT

[LGOM+15] Al Mokhtar Lamsabhi, Soledad Gutiérrez-Oliva, Otilia Mó, Alejandro Toro-Labbé, and Manuel Yáñez. Effects of the ionization in the tautomerism of uracil: a reaction electronic flux perspective. *Journal of Computational Chemistry*, 36(28):2135–2145, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laurent:2014:TUE

[LGVA14] Adèle D. Laurent, Vitaly N. Glushkov, Thibaut Very, and Xavier Assfeld. Toward the understanding of the environmental effects on core ionizations. *Journal of Computational Chemistry*, 35(15):1131–1139, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liang:2012:DFS

[LGW12] Jun-Xi Liang, Zhi-Yuan Geng, and Yong-Cheng Wang. Density functional study of S_N2 substitution reactions for CH_3Cl + $CX^1X^{2\bullet-}$ (X^1 X^2 = HH, HF, HCl, HBr, HI, FF, ClCl, BrBr, and II). *Journal of Computational Chemistry*, 33(6): 595–606, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2011:CAB

[LH11] Chewook Lee and Sihyun Ham. Characterizing amyloid-beta protein misfolding from molecular dynamics simulations with explicit water. *Journal of Computational Chemistry*, 32(2): 349–355, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2014:MDA

[LH14a] Po-Chun Liu and Wei-Ping Hu. The MC-DFT approach including the SCS-MP2 energies to the new minnesota-type functionals. *Journal of Computational Chemistry*, 35(21): 1560–1567, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2014:ASM

[LH14b] Xiao-Jing Liu and Ian Hamilton. Adsorption of small molecules on helical gold nanorods: a relativistic density functional study. *Journal of Computational Chemistry*, 35(27): 1967–1976, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2011:RPS

[LHG11] Matthew S. Lin and Teresa Head-Gordon. Reliable protein structure refinement using a physical energy function. *Journal of Computational Chemistry*, 32(4):709–717, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2014:PDD

[LHHW14] Shu-Shi Li, Cui-Ying Huang, Jiao-Jiao Hao, and Chang-Sheng Wang. A polarizable dipole–dipole interaction model for evaluation of the interaction energies for NH···OC and CH···OC hydrogen-bonded complexes. *Journal of Computational Chemistry*, 35(6):415–426, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2012:SSH

[LHKS12] Xiao-Jing Liu, Ian Hamilton, Robert P. Krawczyk, and Peter Schwerdtfeger. The stability of small helical gold nanorods: a relativistic density functional study. *Journal of Computational Chemistry*, 33(3):311–318, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2010:AUS

[LHL+10] Tzong-Yi Lee, Justin Bo-Kai Hsu, Feng-Mao Lin, Wen-Chi Chang, Po-Chiang Hsu, and Hsien-Da Huang. *N*-Ace: Using solvent accessibility and physicochemical properties to identify protein *N*-acetylation sites. *Journal of Computational Chemistry*, 31(15):2759–2771, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lonsdale:2011:CSW

[LHMM11] Richard Lonsdale, Jeremy N. Harvey, Frederick R. Manby, and Adrian J. Mulholland. Comment on "A stationary-wave model of enzyme catalysis" by Carlo Canepa. *Journal of Computational Chemistry*, 32(2):368–369, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [Can10] and reply [Can11].

Le:2017:IDL

[LHO17] Nguyen-Quoc-Khanh Le, Quang-Thai Ho, and Yu-Yen Ou. Incorporating deep learning with convolutional neural networks and position specific scoring matrices for identifying electron transport proteins. *Journal of Computational Chemistry*, 38(23):2000–2006, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lehtola:2012:SNU

[LHSH12] Jussi Lehtola, Mikko Hakala, Arto Sakko, and Keijo Hämäläinen. Software news and updates: ERKALE — a flexible program package for X-ray properties of atoms and molecules. *Journal of Computational Chemistry*, 33(18):1572–1585, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Loerbroks:2015:SEM

[LHT15] Claudia Loerbroks, Andreas Heimermann, and Walter Thiel. Solvents effects on the mechanism of cellulose hydrolysis: A QM/MM study. *Journal of Computational Chemistry*, 36(15): 1114–1123, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2014:EMI

[Li14a] Xinying Li. Erratum: Metalophilic interaction in gold halide: Quantum chemical study of AuX (X = F–At). *Journal of Computational Chemistry*, 35(22):1664, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [Li14b].

Li:2014:MIG

[Li14b] Xinying Li. Metalophilic interaction in gold halide: Quantum chemical study of AuX (X = F–At). *Journal of Computational Chemistry*, 35(12):923–931, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [Li14a].

Lee:2019:SCM

[LI19] Hui Sun Lee and Wonpil Im. Stalis: a computational method for template-based ab initio ligand design. *Journal of Computational Chemistry*, 40(17):1622–1632, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2018:TSN

[Lin18] Chih-Kai Lin. Theoretical study of nitrogen-doped graphene nanoflakes: Stability and spectroscopy depending on dopant types and flake sizes. *Journal of Computational Chemistry*, 39(20):1387–1397, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Loboda:2016:DQP

[LIRL+16] Oleksandr Loboda, Francesca Ingrosso, Manuel F. Ruiz-López, Heribert Reis, and Claude Millot. Dipole and quadrupole polarizabilities of the water molecule as a function of geometry. *Journal of Computational Chemistry*, 37 (23):2125–2132, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2019:DSN

[LJC+19] Chuan Li, Zhe Jia, Arghya Chakravorty, Swagata Pahari, Yunhui Peng, Sankar Basu, Mahesh Koirala, Shailesh Kumar Panday, Marharyta Petukh, Lin Li, and Emil Alexov. DelPhi Suite: New developments and review of functionalities. *Journal of Computational Chemistry*, 40(28):2502–2508, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luo:2011:TSK

[LJG+11] Jie Luo, Xiujuan Jia, Yang Gao, Guicai Song, Yanbo Yu, Rongshun Wang, and Xiumei Pan. Theoretical study on the kinetics of OH radical reactions with CH_3OOH and CH_3CH_2OOH. *Journal of Computational Chemistry*, 32(6): 987–997, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2011:RBW

[LJL+11] Shao-Yong Lu, Yong-Jun Jiang, Jing Lv, Jian-Wei Zou, and Tian-Xing Wu. Role of bridging water molecules in GSK3β-inhibitor complexes: Insights from QM/MM, MD, and molecular docking studies. *Journal of Computational Chemistry*, 32 (9):1907–1918, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2012:SNU

[LJR+12] Kyu Il Lee, Sunhwan Jo, Huan Rui, Bernhard Egwolf, Benoît Roux, Richard W. Pastor, and Wonpil Im. Software news and updates: Web interface for Brownian dynamics simulation of ion transport and its applications to beta-barrel pores. *Journal of Computational Chemistry*, 33(3):331–339, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:REBa

[LJW11a] Yang Li, Xiao-Nan Jiang, and Chang-Sheng Wang. Rapid evaluation of the binding energies in hydrogen-bonded amide–thymine and amide–uracil dimers in gas phase. *Journal of*

Computational Chemistry, 32(5):953–966, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2011:SSO

[LJW+11b] Ren-Jie Lin, Soonmin Jang, Chen-Chang Wu, Ya-Ling Liu, and Feng-Yin Li. Site specificity of OH α-H abstraction reaction for a β-hairpin peptide: an ab initio study. *Journal of Computational Chemistry*, 32(16):3409–3422, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Latek:2011:CNN

[LK11] Dorota Latek and Andrzej Kolinski. CABS-NMR — de novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. *Journal of Computational Chemistry*, 32(3):536–544, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2013:DSC

[LK13] Han Myoung Lee and Kwang S. Kim. Dynamics and structural changes of small water clusters on ionization. *Journal of Computational Chemistry*, 34(18):1589–1597, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lousada:2016:SCO

[LK16a] Cláudio M. Lousada and Pavel A. Korzhavyi. Surface chemistry of oxygen on aluminum — performance of the density functionals: PBE, PBE0, M06, and M06-L. *Journal of Computational Chemistry*, 37(9):787–794, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lupan:2016:MEI

[LK16b] Alexandru Lupan and R. Bruce King. Molybdatricarbaboranes as examples of isocloso metallaborane deltahedra with three carbon vertices. *Journal of Computational Chemistry*, 37(1):64–69, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2010:DFP

[LKL10] In-Ho Lee, Seung-Yeon Kim, and Jooyoung Lee. Dynamic folding pathway models of the villin headpiece subdomain (HP-36) structure. *Journal of Computational Chemistry*, 31 (1):57–65, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lutz-Kappelman:2018:MOM

[LKZM18] Laura Lutz-Kappelman, Yuemei Zhang, and Gordon J. Miller. Magnetic ordering and metal-atom site preference in tetragonal CrMnAs: Electronic correlation effects. *Journal of Computational Chemistry*, 39(21):1585–1593, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larsson:2010:HPP

[LL10a] Per Larsson and Erik Lindahl. A high-performance parallel-generalized Born implementation enabled by tabulated interaction rescaling. *Journal of Computational Chemistry*, 31(14): 2593–2600, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:MLS

[LL10b] Huameng Li and Chenglong Li. Multiple ligand simultaneous docking: Orchestrated dancing of ligands in binding sites of protein. *Journal of Computational Chemistry*, 31(10):2014–2022, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2010:TDT

[LL10c] J. W. Liu and Z. F. Liu. Thermal dissociation of tripropylamine as the first step in the growth of carbon nanotubes inside $AlPO_4$-5 channels. *Journal of Computational Chemistry*, 31(8):1681–1688, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:TIG

[LL11] Xianfeng Li and Robert A. Latour. The temperature intervals with global exchange of replicas empirical accelerated sampling method: Parameter sensitivity and extension to a complex molecular system. *Journal of Computational Chemistry*, 32(6):1091–1100, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2013:IMD

[LL13a] Yung Ting Lee and Jyh Shing Lin. Ab Initio molecular dynamics study of ethylene adsorption onto Si(001) surface: Short-time Fourier transform analysis of structural coordinate autocorrelation function. *Journal of Computational Chemistry*, 34(31):2697–2706, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2013:EFA

[LL13b] Hongguang Liu and Jin Yong Lee. Electric field assisted oxygen removal from the basal plane of the graphitic material. *Journal of Computational Chemistry*, 34(4):305–310, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lai:2015:ICD

[LL15] Pin-Kuang Lai and Shiang-Tai Lin. Internal coordinate density of state from molecular dynamics simulation. *Journal of Computational Chemistry*, 36(8):507–517, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopes:2019:AAM

[LL19a] Laura J. S. Lopes and Tony Lelièvre. Analysis of the adaptive multilevel splitting method on the isomerization of alanine dipeptide. *Journal of Computational Chemistry*, 40(11):1198–1208, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lubecka:2019:IBP

[LL19b] Emilia A. Lubecka and Adam Liwo. Introduction of a bounded penalty function in contact-assisted simulations of protein structures to omit false restraints. *Journal of Computational Chemistry*, 40(25):2164–2178, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:FPI

[LLB+12] Hongping Li, Shuhui Lv, Yijia Bai, Yanjie Xia, Xiaojuan Liu, and Jian Meng. First-principle investigation of magnetic coupling mechanism in hypothesized A-site-ordered perovskite $YMn_3Sc_4O_{12}$. *Journal of Computational Chemistry*, 33(1): 82–87, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laref:2012:ESX

[LLBO12] A. Laref, S. Laref, and S. Bin-Omran. Electronic structure, X-ray absorption, and optical spectroscopy of $LaCoO_3$ in the ground-state and excited-states. *Journal of Computational Chemistry*, 33(6):673–684, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:EPF

[LLC+10] Xun Li, Yan Li, Tiejun Cheng, Zhihai Liu, and Renxiao Wang. Evaluation of the performance of four molecular docking programs on a diverse set of protein-ligand complexes. *Journal of Computational Chemistry*, 31(11):2109–2125, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2017:NDC

[LLC17] I-Hsiang Lin, Yu-Huan Lu, and Hsin-Tsung Chen. Nitrogen-doped C_{60} as a robust catalyst for CO oxidation. *Journal of Computational Chemistry*, 38(23):2041–2046, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2017:TID

[LLD17] Zhifeng Lin, Tian Lu, and Xun-Lei Ding. A theoretical investigation on doping superalkali for triggering considerable nonlinear optical properties of Si_{12} C_{12} nanostructure. *Journal of Computational Chemistry*, 38(18):1574–1582, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2016:ISV

[LLFH16] Hanzhong Liu, Minghai Li, Jue Fan, and Shuanghong Huo. Inherent structure versus geometric metric for state space discretization. *Journal of Computational Chemistry*, 37(14): 1251–1258, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lii:2011:APE

[LLH11] Jenn-Huei Lii, Fu-Xing Liao, and Ching-Han Hu. Accurate prediction of the enthalpies of formation for xanthophylls. *Journal of Computational Chemistry*, 32(15):3175–3187, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Le:2014:SIK

[LLH14] Thong Nguyen-Minh Le, Bin Liu, and Lam K. Huynh. SurfKin: an ab initio kinetic code for modeling surface reactions. *Journal of Computational Chemistry*, 35(26):1890–1899, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2017:AFD

[LLH17] Kuan-Yu Liu, Jie Liu, and John M. Herbert. Accuracy of finite-difference harmonic frequencies in density functional theory. *Journal of Computational Chemistry*, 38(19):1678–1684, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2019:MFF

[LLH+19] Ke Li, Shanlong Li, Wei Huang, Chunyang Yu, and Yongfeng Zhou. MembrFactory: a force field and composition double independent universal tool for constructing polyamide reverse osmosis membranes. *Journal of Computational Chemistry*, 40 (27):2432–2438, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lakkaraju:2016:DIA

[LLHM16] Sirish Kaushik Lakkaraju, Justin A. Lemkul, Jing Huang, and Alexander D. MacKerell Jr. DIRECT–ID: an automated method to identify and quantify conformational variations — application to β_2-adrenergic GPCR. *Journal of Computational Chemistry*, 37(4):416–425, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Logsdail:2012:DON

[LLJ12] Andrew J. Logsdail, Z. Y. Li, and Roy L. Johnston. Development and optimization of a novel genetic algorithm for identifying nanoclusters from scanning transmission electron microscopy images. *Journal of Computational Chemistry*, 33

(4):391–400, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:NSI

[LLL+10] Jiazhong Li, Shuyan Li, Beilei Lei, Huanxiang Liu, Xiaojun Yao, Mancang Liu, and Paola Gramatica. A new strategy to improve the predictive ability of the local lazy regression and its application to the QSAR study of melanin-concentrating hormone receptor 1 antagonists. *Journal of Computational Chemistry*, 31(5):973–985, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:IBH

[LLL+11] Qingzhong Li, Ran Li, Zhenbo Liu, Wenzuo Li, and Jianbo Cheng. Interplay between halogen bond and lithium bond in MCN–LiCN–XCCH (M = H, Li, and Na; X = Cl, Br, and I) complex: The enhancement of halogen bond by a lithium bond. *Journal of Computational Chemistry*, 32(15): 3296–3303, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lv:2012:IMT

[LLL+12] Shuhui Lv, Xiaojuan Liu, Hongping Li, Lin Han, Zhongchang Wang, and Jian Meng. Insulator–metal transition driven by pressure and B-site disorder in double perovskite La_2CoMnO_6. *Journal of Computational Chemistry*, 33(16): 1433–1439, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liao:2011:NGR

[LLLC11] Bo Liao, Benyou Liao, Xinguo Lu, and Zhi Cao. A novel graphical representation of protein sequences and its application. *Journal of Computational Chemistry*, 32(12):2539–2544, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:FPI

[LLLM11] Hongping Li, Shuhui Lv, Xiaojuan Liu, and Jian Meng. First-principles investigation of A-B intersite charge transfer and correlated electrical and magnetic properties in $BiCu_3Fe_4O_{12}$. *Journal of Computational Chemistry*, 32(7):1235–1240, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2019:URS

[LLLW19] Ping Liu, Lixia Ling, Hao Lin, and Baojun Wang. Understanding the role of surface oxygen in Hg removal on un-doped and Mn/Fe-doped CeO_2 (111). *Journal of Computational Chemistry*, 40(30):2611–2621, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2014:RDM

[LLSW14] Kun Liu, Yu-Xue Li, Jia-Ling Su, and Bin Wang. The reliability of DFT methods to predict electronic structures and minimum energy crossing point for $[Fe^{IV}O](OH)_2$ models: a comparison study with MCQDPT method. *Journal of Computational Chemistry*, 35(9):703–710, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2012:MAD

[LLT12] You Lu, Zhenggang Lan, and Walter Thiel. Monomeric adenine decay dynamics influenced by the DNA environment. *Journal of Computational Chemistry*, 33(13):1225–1235, May 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2012:TDV

[LLTC12] Jyh Shing Lin, Shao-Yu Lu, Po-Jung Tseng, and Wen-Chi Chou. Temperature dependence of vibrational modes of $CH_3CC_{(ads)}$ and $I_{(ads)}$ coadsorbed on Ag(111): ab initio molecular dynamics approach. *Journal of Computational Chemistry*, 33(13):1274–1283, May 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2010:UOS

[LLvG10] Zhixiong Lin, Haiyan Liu, and Wilfred F. van Gunsteren. Using one-step perturbation to predict the effect of changing force-field parameters on the simulated folding equilibrium of a β-peptide in solution. *Journal of Computational Chemistry*, 31(13):2419–2427, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:TCA

[LLW12] Bu-Tong Li, Lu-Lin Li, and Hai-Shun Wu. Theoretical calculation about the valence and Rydberg excited states of hydrogen cyanide. *Journal of Computational Chemistry*, 33(5):

484–489, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liang:2019:DFT

[LLX+19] Yan Ying Liang, Bo Li, Xuan Xu, Feng Long Gu, and Chaoyuan Zhu. A density functional theory study on nonlinear optical properties of double cage excess electron compounds: Theoretically design M [Cu(Ag)@$(NH_3)_n$] (M = Be, Mg and Ca; n = 1–3). *Journal of Computational Chemistry*, 40(9):971–979, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:SNU

[LLZA12] Chuan Li, Lin Li, Jie Zhang, and Emil Alexov. Software news and updates: Highly efficient and exact method for parallelization of grid-based algorithms and its implementation in DelPhi. *Journal of Computational Chemistry*, 33(24):1960–1966, September 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lemkul:2018:PFF

[LM18a] Justin A. Lemkul and Alexander D. MacKerell Jr. Polarizable force field for RNA based on the classical Drude oscillator. *Journal of Computational Chemistry*, 39(32):2624–2646, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez:2018:PMC

[LM18b] Alvaro J. Lopez and Leandro Martínez. Parametric models to compute tryptophan fluorescence wavelengths from classical protein simulations. *Journal of Computational Chemistry*, 39 (19):1249–1258, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Long:2015:GGA

[LMA15] Thomas Long, Owen M. McDougal, and Tim Andersen. GAMPMS: Genetic algorithm managed peptide mutant screening. *Journal of Computational Chemistry*, 36(17):1304–1310, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2014:MUS

[LMI+14] Pai-Chi Li, Naoyuki Miyashita, Wonpil Im, Satoshi Ishido, and Yuji Sugita. Multidimensional umbrella sampling and replica-exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. *Journal of Computational Chemistry*, 35(4):300–308, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Limpanuparb:2014:RCO

[LMR14] Taweetham Limpanuparb, Josh Milthorpe, and Alistair P. Rendell. Resolutions of the Coulomb operator: VIII. Parallel implementation using the modern programming language X10. *Journal of Computational Chemistry*, 35(28):2056–2069, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lettieri:2011:EFB

[LMZ11a] Steven Lettieri, Artem B. Mamonov, and Daniel M. Zuckerman. Extending fragment-based free energy calculations with library Monte Carlo simulation: Annealing in interaction space. *Journal of Computational Chemistry*, 32(6):1135–1143, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:SAD

[LMZ+11b] Chun Li, Hong Ma, Yang Zhou, Xiaolei Wang, and Xiaoqi Zheng. Similarity analysis of DNA sequences based on the weighted pseudo-entropy. *Journal of Computational Chemistry*, 32(4):675–680, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lime:2015:IQM

[LN15] Elaine Limé and Per-Ola Norrby. Improving the Q2MM method for transition state force field modeling. *Journal of Computational Chemistry*, 36(4):244–250, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laun:2018:CGB

[LOB18] Joachim Laun, Daniel Vilela Oliveira, and Thomas Bredow. Consistent Gaussian basis sets of double- and triple-zeta valence with polarization quality of the fifth period for solid-state calculations. *Journal of Computational Chemistry*, 39 (19):1285–1290, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laoui:2011:WSA

[LP11a] Abdel Laoui and Valery R. Polyakov. Web services as applications' integration tool: QikProp case study. *Journal of Computational Chemistry*, 32(9):1944–1951, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2011:ESF

[LP11b] Bin Lin and B. Montgomery Pettitt. Electrostatic solvation free energy of amino acid side chain analogs: Implications for the validity of electrostatic linear response in water. *Journal of Computational Chemistry*, 32(5):878–885, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luchow:2011:SED

[LP11c] Arne Lüchow and René Petz. Single electron densities: a new tool to analyze molecular wavefunctions. *Journal of Computational Chemistry*, 32(12):2619–2626, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Labat:2011:RNE

[LPAS11] Frédéric Labat, Claude Pouchan, Carlo Adamo, and Gustavo E. Scuseria. Role of nonlocal exchange in molecular crystals: the case of two proton-ordered phases of ice. *Journal of Computational Chemistry*, 32(10):2177–2185, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lim:2010:TDS

[LPE+10] Len Herald V. Lim, Andreas B. Pribil, Andreas E. Ellmerer, Bernhard R. Randolf, and Bernd M. Rode. Temperature dependence of structure and dynamics of the hydrated Ca^{2+} ion according to ab initio quantum mechanical charge field and classical molecular dynamics. *Journal of Computational Chemistry*, 31(6):1195–1200, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2016:PGA

[LPK16] Youhan Lee, Roberta Poloni, and Jihan Kim. Probing gas adsorption in MOFs using an efficient ab initio Widom insertion Monte Carlo method. *Journal of Computational Chemistry*, 37(32):2808–2815, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2013:CDS

[LPLA13] Chuan Li, Marharyta Petukh, Lin Li, and Emil Alexov. Continuous development of schemes for parallel computing of the electrostatics in biological systems: Implementation in DelPhi. *Journal of Computational Chemistry*, 34(22):1949–1960, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lombardi:2016:ETD

[LPLB16] Andrea Lombardi, Fernando Pirani, Antonio Laganà, and Massimiliano Bartolomei. Energy transfer dynamics and kinetics of elementary processes (promoted) by gas-phase CO_2–N_2 collisions: Selectivity control by the anisotropy of the interaction. *Journal of Computational Chemistry*, 37(16):1463–1475, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lei:2016:CDA

[LPLS16] Shulai Lei, Beate Paulus, Shujuan Li, and Burkhard Schmidt. Curvature-dependent adsorption of water inside and outside armchair carbon nanotubes. *Journal of Computational Chemistry*, 37(14):1313–1320, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ly:2017:DFT

[LPMT17] Uyen Q. Ly, My-Phuong Pham, Maurice J. Marks, and Thanh N. Truong. Density functional theory study of mechanism of epoxy-carboxylic acid curing reaction. *Journal of Computational Chemistry*, 38(14):1093–1102, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Largent:2012:SNU

[LPS12] R. Jeffrey Largent, William F. Polik, and J. R. Schmidt. Software news and updates: Symmetrizer: Algorithmic determination of point groups in nearly symmetric molecules. *Journal of Computational Chemistry*, 33(19):1637–1642, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2013:PSS

[LPS+13] Xinbi Li, Sergei Y. Ponomarev, Qina Sa, Daniel L. Sigalovsky, and George A. Kaminski. Polarizable simulations with second order interaction model (POSSIM) force field: Developing parameters for protein side-chain analogues. *Journal of Computational Chemistry*, 34(14):1241–1250, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lasinski:2012:RPI

[LRBB12] Michael E. Lasinski, Nichols A. Romero, Shawn T. Brown, and Jean-Philippe Blaudeau. Recent performance improvements to the DFT and TDDFT in GAMESS. *Journal of Computational Chemistry*, 33(7):723–731, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez:2013:IPE

[LRER13] Rafael López, Guillermo Ramírez, Ignacio Ema, and Jaime Fernández Rico. Improved partition–expansion of two-center distributions involving Slater functions. *Journal of Computational Chemistry*, 34(21):1800–1809, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lemkul:2015:SNU

[LRvdSM15] Justin A. Lemkul, Benoît Roux, David van der Spoel, and Alexander D. MacKerell Jr. Software news and updates: Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. *Journal of Computational Chemistry*, 36(19):1473–1479, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lervik:2017:SNU

[LRvE17] Anders Lervik, Enrico Riccardi, and Titus S. van Erp. Software news and updates: PyRETIS: a well-done, medium-sized Python library for rare events. *Journal of Computational*

Chemistry, 38(28):2439–2451, October 30, 2017. CODEN JC-CHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lara:2018:PCM

[LRVM18] A. Lara, M. Riquelme, and E. Vöhringer-Martinez. Partition coefficients of methylated DNA bases obtained from free energy calculations with molecular electron density derived atomic charges. *Journal of Computational Chemistry*, 39(22): 1728–1737, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Launay:2011:LDS

[LS11a] Guillaume Launay and Thomas Simonson. A large decoy set of protein–protein complexes produced by flexible docking. *Journal of Computational Chemistry*, 32(1):106–120, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2011:EGS

[LS11b] Yang Liu and Huai Sun. Electronic ground states and vibrational frequency shifts of diatomic ligands in heme adducts. *Journal of Computational Chemistry*, 32(7):1279–1285, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lei:2010:NIM

[LSD+10] Yibo Lei, Bingbing Suo, Yusheng Dou, Yubin Wang, and Zhenyi Wen. New implementations of MRCI in semiempirical frameworks. *Journal of Computational Chemistry*, 31(8): 1752–1758, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2011:ATD

[LSH+11] Wenlan Liu, Volker Settels, Philipp H. P. Harbach, Andreas Dreuw, Reinhold F. Fink, and Bernd Engels. Assessment of TD-DFT- and TD-HF-based approaches for the prediction of exciton coupling parameters, potential energy curves, and electronic characters of electronically excited aggregates. *Journal of Computational Chemistry*, 32(9):1971–1981, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laloo:2019:EFA

[LSL+19] Jalal Z. A. Laloo, Nandini Savoo, Nassirah Laloo, Lydia Rhyman, and Ponnadurai Ramasami. ExcelAutomat 1.3: Fragment analysis based on the distortion/interaction-activation strain model. *Journal of Computational Chemistry*, 40(3): 619–624, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liao:2013:CQO

[LT13] Rong-Zhen Liao and Walter Thiel. Convergence in the QM-only and QM/MM modeling of enzymatic reactions: a case study for acetylene hydratase. *Journal of Computational Chemistry*, 34(27):2389–2397, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2014:OAC

[LT14] Haining Liu and C. Heath Turner. Oxygen adsorption characteristics on hybrid carbon and boron-nitride nanotubes. *Journal of Computational Chemistry*, 35(14):1058–1063, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Long:2011:CSU

[LTA+11] Stephen M. Long, Tran T. Tran, Peter Adams, Paul Darwen, and Mark L. Smythe. Conformational searching using a population-based incremental learning algorithm. *Journal of Computational Chemistry*, 32(8):1541–1549, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2011:IMO

[LTP11] Zhiwei Liu, Alexey Teslja, and Vojislava Pophristic. An ab initio molecular orbital study of intramolecular hydrogen bonding in ortho-substituted arylamides: Implications for the parameterization of molecular mechanics force fields. *Journal of Computational Chemistry*, 32(9):1846–1858, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2018:MSF

[LTR18] Jingbai Li, Divya Tadakamalla, and Andrey Yu. Rogachev. Modulating stability of functionalized fullerene cations [R-

$C_60]^+$ with the nature of R-group. *Journal of Computational Chemistry*, 39(28):2385–2396, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lamiable:2016:CAH

[LTT16] A. Lamiable, P. Thevenet, and P. Tufféry. A critical assessment of hidden Markov model sub-optimal sampling strategies applied to the generation of peptide 3D models. *Journal of Computational Chemistry*, 37(21):2006–2016, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2011:CSS

[Lu11] Shih-I Lu. Computational study of static first hyperpolarizability of donor–acceptor substituted (E)-benzaldehyde phenylhydrazone. *Journal of Computational Chemistry*, 32 (4):730–736, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luchow:2014:MCB

[Lüc14] Arne Lüchow. Maxima of —Ψ —2: a connection between quantum mechanics and Lewis structures. *Journal of Computational Chemistry*, 35(11):854–864, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lundberg:2012:UCB

[Lun12] Marcus Lundberg. Understanding cross-boundary events in ONIOM QM:QM' calculations. *Journal of Computational Chemistry*, 33(4):406–415, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larsson:2013:GOP

[LvDH13] Henrik R. Larsson, Adri C. T. van Duin, and Bernd Hartke. Global optimization of parameters in the reactive force field ReaxFF for SiOH. *Journal of Computational Chemistry*, 34 (25):2178–2189, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2013:IVS

[LvG13a] Zhixiong Lin and Wilfred F. van Gunsteren. Influence of variation of a side chain on the folding equilibrium of a β-peptide:

Limitations of one-step perturbation. *Journal of Computational Chemistry*, 34(22):1899–1906, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2013:CRS

[LvG13b] Zhixiong Lin and Wilfred F. van Gunsteren. On the choice of a reference state for one-step perturbation calculations between polar and nonpolar molecules in a polar environment. *Journal of Computational Chemistry*, 34(5):387–393, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2013:RAG

[LvG13c] Zhixiong Lin and Wilfred F. van Gunsteren. Refinement of the application of the GROMOS 54A7 force field to β-peptides. *Journal of Computational Chemistry*, 34(32):2796–2805, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:REBb

[LW11] Yang Li and Chang-Sheng Wang. Rapid evaluation of the binding energies between peptide amide and DNA base. *Journal of Computational Chemistry*, 32(13):2765–2773, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Landis:2016:ERH

[LW16] C. R. Landis and F. Weinhold. 18-electron rule and the 3c/4e hyperbonding saturation limit. *Journal of Computational Chemistry*, 37(2):237–241, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2013:QWP

[LWD13] Ruifeng Lu, Yunhui Wang, and Kaiming Deng. Quantum wave packet and quasiclassical trajectory studies of the reaction H(^{2}S) + CH(X$^2\Pi$); $v = 0$, j = 1 $\rightarrow$ C(^{1} D) + H$_2$ (X$^1\Sigma$ g+): Coriolis coupling effects and stereodynamics. *Journal of Computational Chemistry*, 34(20):1735–1742, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2015:CCI

[LWGZ15] Yuanyuan Li, Li Wang, Xugeng Guo, and Jinglai Zhang. A CASSCF/CASPT2 insight into excited-state intramolecular proton transfer of four imidazole derivatives. *Journal of Computational Chemistry*, 36(32):2374–2380, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larsen:2014:GMI

[LWK+14] Adrien B. Larsen, Jeffrey R. Wagner, Saugat Kandel, Romelia Salomon-Ferrer, Nagarajan Vaidehi, and Abhinandan Jain. GneimoSim: a modular internal coordinates molecular dynamics simulation package. *Journal of Computational Chemistry*, 35(31):2245–2255, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2010:APE

[LWL+10] Cun-Xi Liu, Hai-Xia Wang, Ze-Rong Li, Chong-Wen Zhou, Han-Bing Rao, and Xiang-Yuan Li. Accurate prediction of enthalpies of formation for a large set of organic compounds. *Journal of Computational Chemistry*, 31(14):2585–2592, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:TSP

[LWL+11] Xiao-Na Li, Zhi-Jian Wu, Xi-Yan Li, Hong-Jie Zhang, and Xiao-Juan Liu. Theoretical study on phosphorescence efficiency and color tuning from orange to blue-green of Ir(III) complexes based on substituted 2-phenylimidazo[1,2-a]pyridine ligand. *Journal of Computational Chemistry*, 32(6):1033–1042, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2016:RBB

[LWL+16] Guoliang Li, Hui Wang, Qian-Shu Li, Yaoming Xie, and Henry F. Schaefer III. The reaction between bromine and the water dimer and the highly exothermic reverse reaction. *Journal of Computational Chemistry*, 37(2):177–182, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:VRE

[LWW12] Bu-Tong Li, Zi-Zhang Wei, and Hai-Shun Wu. The valence and Rydberg excited states of CH_2: a theoretical exploration. *Journal of Computational Chemistry*, 33(31):2498–2503, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2012:TIS

[LWWG12] Hui Liu, Fang Wang, Gui-Xiang Wang, and Xue-Dong Gong. Theoretical investigations on structure, density, detonation properties, and sensitivity of the derivatives of PYX. *Journal of Computational Chemistry*, 33(22):1790–1796, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2016:TSP

[LWXC16] Li-Hong Liu, Dan Wu, Shu-Hua Xia, and Ganglong Cui. Theoretical study on photooxidation mechanism of ruthenium complex $[Ru(II)\text{-}(bpy)_2\ (TMBiimH_2)]^{2+}$ with molecular oxygen. *Journal of Computational Chemistry*, 37(24):2212–2219, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2017:SNU

[LWZ+17] Beibei Liu, Bao Wang, Rundong Zhao, Yiying Tong, and Guo-Wei Wei. Software news and updates: ESES: Software for Eulerian solvent excluded surface. *Journal of Computational Chemistry*, 38(7):446–466, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2019:RMN

[LWZ+19] Hui Li, Di Wang, Xin Zhao, Li-Nan Lu, Cui Liu, Li-Dong Gong, Dong-Xia Zhao, and Zhong-Zhi Yang. Reaction mechanism of NO with hydrolysates of NAMI-A: an MD simulation by combining the QM/ MM(ABEEM) with the MD-FEP method. *Journal of Computational Chemistry*, 40(10):1141–1150, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2013:MRT

[LWZK13] Hongmei Liu, Hongbo Wang, Jianwei Zhao, and Manabu Kiguchi. Molecular rectification in triangularly shaped graphene nanoribbons. *Journal of Computational Chemistry*, 34(5):360–365, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2011:NIP

[LX11] Sen Lin and Daiqian Xie. New ab initio potential energy surfaces for both the ground ($\tilde{X}^1A'$) and excited ($\tilde{A}^1A''$) electronic states of HSiCl and the absorption and emission spectra of HSiCl/DSiCl. *Journal of Computational Chemistry*, 32(8):1694–1702, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2017:TSS

[LXFC17] Xiang-Yang Liu, Pin Xiao, Wei-Hai Fang, and Ganglong Cui. Theoretical studies of spin state-specific [2 + 2] and [5 + 2] photocycloaddition reactions of *n*-(1-penten-5-yl)maleimide. *Journal of Computational Chemistry*, 38(28):2388–2395, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:SPD

[LXL+11] Shuyan Li, Lili Xi, Jiazhong Li, Chengqi Wang, Beilei Lei, Yulin Shen, Huanxiang Liu, Xiaojun Yao, and Biao Li. In silico prediction of deleterious single amino acid polymorphisms from amino acid sequence. *Journal of Computational Chemistry*, 32(7):1211–1216, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2010:DTD

[LXZ+10] Tao Liu, Bao-Hui Xia, Qing-Chuan Zheng, Xin Zhou, Qing-Jiang Pan, and Hong-Xing Zhang. DFT/TD-DFT investigation on Ir(III) complexes with *N*-heterocyclic carbene ligands: Geometries, electronic structures, absorption, and phosphorescence properties. *Journal of Computational Chemistry*, 31 (3):628–638, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lankau:2010:MSE

[LY10] Timm Lankau and Chin-Hui Yu. A model study of the efficiency of the Asp–His–Ser triad. *Journal of Computational Chemistry*, 31(9):1853–1859, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2013:ADM

[LYC+13] Yongqing Li, Jiuchuang Yuan, Maodu Chen, Fengcai Ma, and Mengtao Sun. Accurate double many-body expansion potential energy surface by extrapolation to the complete basis set limit and dynamics calculations for ground state of NH_2. *Journal of Computational Chemistry*, 34(19):1686–1696, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2016:NSB

[LYL16] Xiaojun Li, Zhijun Yan, and Shuna Li. The nature of structure and bonding between transition metal and mixed Si — Ge tetramers: a 20-electron superatom system. *Journal of Computational Chemistry*, 37(25):2316–2323, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2011:TDS

[LYSS11] Yu-Fang Liu, Da-Peng Yang, De-Heng Shi, and Jin-Feng Sun. A TD-DFT study on the hydrogen bonding of three esculetin complexes in electronically excited states: Strengthening and weakening. *Journal of Computational Chemistry*, 32(16):3475–3484, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Leis:2011:EIR

[LZ11] Simon Leis and Martin Zacharias. Efficient inclusion of receptor flexibility in grid-based protein–ligand docking*. *Journal of Computational Chemistry*, 32(16):3433–3439, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lettieri:2012:AMM

[LZ12] Steven Lettieri and Daniel M. Zuckerman. Accelerating molecular Monte Carlo simulations using distance and orientation-dependent energy tables: Tuning from atomistic accuracy to smoothed "coarse-grained" models. *Journal of Computational Chemistry*, 33(3):268–275, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2014:MSP

[LZ14] Wenliang Li and Jingping Zhang. Multiscale simulation of pollution gases adsorption in porous organic cage CC3. *Journal of Computational Chemistry*, 35(2):174–180, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2018:SBS

[LZ18] M. W. Li and P. M. Zimmerman. Stepwise basis set selection. *Journal of Computational Chemistry*, 39(26):2153–2162, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lev:2010:QMI

[LZdlL+10] Bogdan Lev, Rui Zhang, Aurélien de la Lande, Dennis Salahub, and Sergei Yu Noskov. The QM–MM interface for CHARMM–deMon. *Journal of Computational Chemistry*, 31 (5):1015–1023, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liang:2011:PSC

[LZGS11] Shide Liang, Yaoqi Zhou, Nick Grishin, and Daron M. Standley. Protein side chain modeling with orientation-dependent atomic force fields derived by series expansions. *Journal of Computational Chemistry*, 32(8):1680–1686, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:ICC

[LZH+11] Huifang Li, Laibin Zhang, Li Han, Wenming Sun, and Yuxiang Bu. Internucleotide J-couplings and chemical shifts of the $\mathrm{N} - \mathrm{H} \cdots \mathrm{N}$ hydrogen-bonds in the radiation-damaged guanine-cytosine base pairs. *Journal of Computational Chemistry*, 32(6):1159–1169, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Levandowski:2016:SHA

[LZH16] Brian J. Levandowski, Lufeng Zou, and K. N. Houk. Schleyer hyperconjugative aromaticity and Diels–Alder reactivity of 5-substituted cyclopentadienes. *Journal of Computational Chemistry*, 37(1):117–123, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:TDS

[LZHH11] Guang-Yue Li, Guang-Jiu Zhao, Ke-Li Han, and Guo-Zhong He. A TD-DFT study on the cyanide-chemosensing mechanism of 8-formyl-7-hydroxycoumarin. *Journal of Computational Chemistry*, 32(4):668–674, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2011:SPN

[LZJ+11] Qing-Zhong Li, Jun-Ling Zhao, Bo Jing, Ran Li, Wen-Zuo Li, and Jian-Bo Cheng. The structure, properties, and nature of HArF–HOX (X = F, Cl, Br) complex: an ab initio study and an unusual short hydrogen bond. *Journal of Computational Chemistry*, 32(11):2432–2440, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2010:TDS

[LZL+10] Guang-Yue Li, Guang-Jiu Zhao, Yu-Hui Liu, Ke-Li Han, and Guo-Zhong He. TD–DFT study on the sensing mechanism of a fluorescent chemosensor for fluoride: Excited-state proton transfer. *Journal of Computational Chemistry*, 31(8):1759–1765, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2013:FNM

[LZL+13] Yu Liu, Lei Zhao, Wentao Li, Dongyu Zhao, Miao Song, and Yongliang Yang. FIPSDock: a new molecular docking technique driven by fully informed swarm optimization algorithm. *Journal of Computational Chemistry*, 34(1):67–75, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2015:CQM

[LZL+15a] Hongzhi Li, Ziyan Zhong, Lin Li, Rui Gao, Jingxia Cui, Ting Gao, Li Hong Hu, Yinghua Lu, Zhong-Min Su, and Hui Li. A cascaded QSAR model for efficient prediction of overall power conversion efficiency of all-organic dye-sensitized solar cells. *Journal of Computational Chemistry*, 36(14):1036–1046, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2015:CXH

[LZL+15b] Wei Li, Yanli Zeng, Xiaoyan Li, Zheng Sun, and Lingpeng Meng. The competition of Y · O and X · N halogen bonds to enhance the group V σ-hole interaction in the NCY · o PH_3 · NCX and O PH_3 · NCX · NCY (X, Y F, Cl, and Br) complexes. *Journal of Computational Chemistry*, 36(18): 1349–1358, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2016:MIM

[LZL+16] Jiahui Liu, Yiying Zheng, Ying Liu, Haiyan Yuan, and Jingping Zhang. Mechanistic insight on (E)-methyl 3-(2-aminophenyl)acrylate cyclization reaction by multicatalysis of solvent and substrate. *Journal of Computational Chemistry*, 37(26):2386–2394, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2013:ADI

[LZLC13] Yuan Liu, Jijun Zhao, Fengyu Li, and Zhongfang Chen. Appropriate description of intermolecular interactions in the methane hydrates: an assessment of DFT methods. *Journal of Computational Chemistry*, 34(2):121–131, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2016:KCG

[LZLMP16] Hong Liu, You-Liang Zhu, Zhong-Yuan Lu, and Florian Müller-Plathe. A kinetic chain growth algorithm in coarse-grained simulations. *Journal of Computational Chemistry*, 37(30):2634–2646, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2017:APL

[LZS+17] Song Liu, Lizhe Zhu, Fu Kit Sheong, Wei Wang, and Xuhui Huang. Adaptive partitioning by local density-peaks: an efficient density-based clustering algorithm for analyzing molecular dynamics trajectories. *Journal of Computational Chemistry*, 38(3):152–160, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2019:PHS

[LZSM19] Mengyu Liu, Yanli Zeng, Zheng Sun, and Lingpeng Meng. Predicting the halogen- n (n = 3-6) synthons to form the “windmill” pattern bonding based on the halogen-bonded interactions. *Journal of Computational Chemistry*, 40(11): 1219–1226, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larin:2010:IEB

[LZTV10] A. V. Larin, G. M. Zhidomirov, D. N. Trubnikov, and D. P. Vercauteren. Ion-exchanged binuclear Ca_2O_x clusters, $x = 1$–4, as active sites of selective oxidation over MOR and FAU zeolites. *Journal of Computational Chemistry*, 31(2):421–430, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2011:CTT

[LZW+11] Hongmei Liu, Zhenzhen Zhao, Nan Wang, Cui Yu, and Jianwei Zhao. Can the transition from tunneling to hopping in molecular junctions be predicted by theoretical calculation? *Journal of Computational Chemistry*, 32(8):1687–1693, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2016:NAC

[LZX16] Min Li, John Z. H. Zhang, and Fei Xia. A new algorithm for construction of coarse-grained sites of large biomolecules. *Journal of Computational Chemistry*, 37(9):795–804, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2012:TIT

[LZY+12a] Jinliang Li, Zhenzhen Zhao, Cui Yu, Hongbo Wang, and Jianwei Zhao. Theoretical investigation on the transportation behavior of molecular wires with redox reaction. *Journal of Computational Chemistry*, 33(6):666–672, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2012:DEI

[LZY12b] Cui Liu, Dong-Xia Zhao, and Zhong-Zhi Yang. Direct evaluation of individual hydrogen bond energy in situ in intraand intermolecular multiple hydrogen bonds system. *Journal of Computational Chemistry*, 33(4):379–390, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Legenski:2011:FFM

[LZZ+11] Nicole Legenski, Chenggang Zhou, Qingfan Zhang, Bo Han, Jinping Wu, Liang Chen, Hansong Cheng, and Robert C. Forrey. Force fields for metallic clusters and nanoparticles. *Journal of Computational Chemistry*, 32(8):1711–1720, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liang:2014:LHA

[LZZ14] Shide Liang, Chi Zhang, and Yaoqi Zhou. LEAP: Highly accurate prediction of protein loop conformations by integrating coarse-grained sampling and optimized energy scores with all-atom refinement of backbone and side chains. *Journal of Computational Chemistry*, 35(4):335–341, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez-Araya:2016:GOF

[MA16] Jorge I. Martínez-Araya. A generalized operational formula based on total electronic densities to obtain 3D pictures of the dual descriptor to reveal nucleophilic and electrophilic sites accurately on closed-shell molecules. *Journal of Computational Chemistry*, 37(25):2279–2303, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezey:2017:ASP

[MA17] Paul G. Mezey and Zoltan Antal. An alternative to the "Star Path" enhancement of the ADMA linear scaling method for protein modeling. *Journal of Computational Chemistry*, 38 (20):1774–1779, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Michaud-Agrawal:2011:MTA

[MADWB11] Naveen Michaud-Agrawal, Elizabeth J. Denning, Thomas B. Woolf, and Oliver Beckstein. MDAnalysis: a toolkit for the analysis of molecular dynamics simulations. *Journal of Computational Chemistry*, 32(10):2319–2327, July 30, 2011. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matanovic:2014:ADF

[MAK+14] Ivana Matanović, Plamen Atanassov, Boris Kiefer, Fernando H. Garzon, and Neil J. Henson. Applicability of density functional theory in reproducing accurate vibrational spectra of surface bound species. *Journal of Computational Chemistry*, 35(26):1921–1929, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mironov:2019:SSM

[MAMF19] Vladimir Mironov, Yuri Alexeev, Vikram Khipple Mulligan, and Dmitri G. Fedorov. A systematic study of minima in alanine dipeptide. *Journal of Computational Chemistry*, 40 (2):297–309, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manz:2013:LEC

[Man13] Thomas A. Manz. Letters to the Editor: Comment on "Extending Hirshfeld-I to bulk and periodic materials". *Journal of Computational Chemistry*, 34(5):418–421, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [VBV13a, VVB13].

Manak:2019:VBD

[Man19a] Martin Manak. Voronoi-based detection of pockets in proteins defined by large and small probes. *Journal of Computational Chemistry*, 40(19):1758–1771, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manogaran:2019:MBS

[Man19b] Dhivya Manogaran. Making and breaking of small water clusters: a combined quantum chemical and molecular dynamics approach. *Journal of Computational Chemistry*, 40(16):1556–1569, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitchell:2018:DFT

[MAP18] Izaac Mitchell, Bálint Aradi, and Alister J. Page. Density functional tight binding-based free energy simulations in the DFTB+ program. *Journal of Computational Chemistry*, 39

(29):2452–2458, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mehdi:2010:ESR

[MAPB10] Ahmed Mehdi, Legesse Adane, Dhilon S. Patel, and Prasad V. Bharatam. Electronic structure and reactivity of guanylthiourea: a quantum chemical study. *Journal of Computational Chemistry*, 31(6):1259–1267, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matta:2010:HDM

[Mat10] Chérif F. Matta. How dependent are molecular and atomic properties on the electronic structure method? Comparison of Hartree–Fock, DFT, and MP2 on a biologically relevant set of molecules. *Journal of Computational Chemistry*, 31(6):1297–1311, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matta:2014:MBB

[Mat14] Chérif F. Matta. Modeling biophysical and biological properties from the characteristics of the molecular electron density, electron localization and delocalization matrices, and the electrostatic potential. *Journal of Computational Chemistry*, 35 (16):1165–1198, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matta:2018:QCI

[Mat18] Chérif F. Matta. Quantum crystallography: From the intersection to the union of crystallography and quantum mechanics. *Journal of Computational Chemistry*, 39(17):1019–1020, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maurice:2014:STF

[Mau14] Kevin J. Maurice. SSThread: Template-free protein structure prediction by threading pairs of contacting secondary structures followed by assembly of overlapping pairs. *Journal of Computational Chemistry*, 35(8):644–656, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mogo:2014:SNU

[MB14] César Mogo and João Brandão. Software news and updates: The READY program: Building a global potential energy surface and reactive dynamic simulations for the hydrogen combustion. *Journal of Computational Chemistry*, 35(17):1330–1337, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mogo:2016:SNU

[MB16] César Mogo and João Brandão. Software news and updates: N-dimensional switch function for energy conservation in multiprocess reaction dynamics. *Journal of Computational Chemistry*, 37(16):1521–1524, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manzin:2011:ATS

[MBA11] Alessandra Manzin, Oriano Bottauscio, and Domenico Patrizio Ansalone. Application of the thin-shell formulation to the numerical modeling of Stern layer in biomolecular electrostatics. *Journal of Computational Chemistry*, 32(14):3105–3113, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohammed:2014:DRP

[MBA14] Ahmed A. K. Mohammed, Steven K. Burger, and Paul W. Ayers. Drug release by pH-responsive molecular tweezers: Atomistic details from molecular modeling. *Journal of Computational Chemistry*, 35(21):1545–1551, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masella:2011:CPF

[MBC11] Michel Masella, Daniel Borgis, and Philippe Cuniasse. Combining a polarizable force-field and a coarse-grained polarizable solvent model. II. Accounting for hydrophobic effects. *Journal of Computational Chemistry*, 32(12):2664–2678, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masella:2013:MCG

[MBC13] Michel Masella, Daniel Borgis, and Philippe Cuniasse. A multiscale coarse-grained polarizable solvent model for handling long tail bulk electrostatics. *Journal of Computational Chemistry*, 34(13):1112–1124, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohamed:2016:ESF

[MBE16] Noor Asidah Mohamed, Richard T. Bradshaw, and Jonathan W. Essex. Evaluation of solvation free energies for small molecules with the AMOEBA polarizable force field. *Journal of Computational Chemistry*, 37(32):2749–2758, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mondal:2015:DEO

[MBFG15] Krishnakanta Mondal, Arup Banerjee, Alessandro Fortunelli, and Tapan K. Ghanty. Does enhanced oxygen activation always facilitate CO oxidation on gold clusters? *Journal of Computational Chemistry*, 36(29):2177–2187, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Menendez:2015:OEI

[MBFP15] Marcos Menéndez, Roberto Álvarez Boto, Evelio Francisco, and Ángel Martín Pendás. One-electron images in real space: Natural adaptive orbitals. *Journal of Computational Chemistry*, 36(11):833–843, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez:2015:SNU

[MBR+15] Michael Martinez, Neil J. Bruce, Julia Romanowska, Daria B. Kokh, Musa Ozboyaci, Xiaofeng Yu, Mehmet Ali Öztürk, Stefan Richter, and Rebecca C. Wade. Software news and updates: SDA 7: a modular and parallel implementation of the simulation of diffusional association software. *Journal of Computational Chemistry*, 36(21):1631–1645, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Moreira:2016:QMC

[MBRC16] N. L. Moreira, B. G. A. Brito, J. N. Teixeira Rabelo, and Ladir Cândido. Quantum Monte Carlo study of the energetics of small hydrogenated and fluoride lithium clusters. *Journal of Computational Chemistry*, 37(17):1531–1536, June 30,

2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maciejewski:2014:DCD

[MBT14] Mateusz Maciejewski, Paul N. Barlow, and Nico Tjandra. Decoding the components of dynamics in three-domain proteins. *Journal of Computational Chemistry*, 35(7):518–525, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mandado:2010:SMA

[MC10] Marcos Mandado and M. Natália D. S. Cordeiro. On the stability of metal–aminoacid complexes in water based on water–ligand exchange reactions and electronic properties: Detailed study on iron–glycine hexacoordinated complexes. *Journal of Computational Chemistry*, 31(15):2735–2745, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahapatra:2012:DPS

[MC12] Uttam Sinha Mahapatra and Sudip Chattopadhyay. Diagnosis of the performance of the state-specific multireference coupled-cluster method with different truncation schemes. *Journal of Computational Chemistry*, 33(14):1285–1303, May 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mendoza-Cortes:2016:PCP

[MCAG+16] Jose L. Mendoza-Cortes, Qi An, William A. Goddard III, Caichao Ye, and Sergey Zybin. Prediction of the crystal packing of di-tetrazine-tetroxide (DTTO) energetic material. *Journal of Computational Chemistry*, 37(2):163–167, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muz:2015:SGM

[MCAY15] İskender Muz, Osman Canko, Murat Atiş, and Erdem Kamil Yıldırım. Search for the global minimum structures of AlB_3H_{2n} ($n = 0$–6) clusters. *Journal of Computational Chemistry*, 36(6):385–391, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahapatra:2011:SOS

[MCC11] Uttam Sinha Mahapatra, Sudip Chattopadhyay, and Rajat K. Chaudhuri. Second-order state-specific multireference Møller–Plesset perturbation theory: Application to energy surfaces of diimide, ethylene, butadiene, and cyclobutadiene. *Journal of Computational Chemistry*, 32(2):325–337, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mooney:2012:MIG

[MCC12] Barbara Logan Mooney, L. René Corrales, and Aurora E. Clark. MoleculaRnetworks: an integrated graph theoretic and data mining tool to explore solvent organization in molecular simulation. *Journal of Computational Chemistry*, 33(8):853–860, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martorell:2010:FPS

[MCF10] Benjamí Martorell, Anna Clotet, and Jordi Fraxedas. A first principle study of the structural, vibrational and electronic properties of tetrathiafulvalene adsorbed on Ag(110) and Au(110) surfaces. *Journal of Computational Chemistry*, 31(9):1842–1852, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maschietto:2018:HCT

[MCF+18] Federica Maschietto, Marco Campetella, Michael J. Frisch, Giovanni Scalmani, Carlo Adamo, and Ilaria Ciofini. How are the charge transfer descriptors affected by the quality of the underpinning electronic density? *Journal of Computational Chemistry*, 39(12):735–742, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Munoz-Castro:2017:EBE

[MCK17a] Alvaro Muñoz-Castro and R. Bruce King. Evaluation of bonding, electron affinity, and optical properties of $M@C_{28}$ (M = Zr, Hf, Th, and U): Role of *d*- and *f*-orbitals in endohedral fullerenes from relativistic DFT calculations. *Journal of Computational Chemistry*, 38(1):44–50, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Munoz-Castro:2017:FSB

[MCK17b] Alvaro Muñoz-Castro and R. Bruce King. On the formation of smaller p-block endohedral fullerenes: Bonding analysis in the $E@C_{20}$ (E = Si, Ge, Sn, Pb) series from relativistic DFT calculations. *Journal of Computational Chemistry*, 38(19): 1661–1667, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mok:2010:HLI

[MCLD10] Daniel K. W. Mok, Foo-Tim Chau, Edmond P. F. Lee, and John M. Dyke. High-level ab initio calculations on HGeCl and the equilibrium geometry of the $\tilde{A}^1A'$ state derived from Franck–Condon analysis of the single-vibronic-level emission spectra of HGeCl and DGeCl. *Journal of Computational Chemistry*, 31(3):476–491, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Murphy:2018:DSO

[MCP18] Paul Murphy, Jeremy P. Coe, and Martin J. Paterson. Development of spin-orbit coupling for stochastic configuration interaction techniques. *Journal of Computational Chemistry*, 39(6):319–327, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martins-Costa:2017:RMN

[MCRL17] Marilia T. C. Martins-Costa and Manuel F. Ruiz-López. Reaching multi-nanosecond timescales in combined QM/MM molecular dynamics simulations through parallel horsetail sampling. *Journal of Computational Chemistry*, 38(10):659–668, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2011:IDP

[MCS11] Zhinan Ma, Wensheng Cai, and Xueguang Shao. Impact of different potentials on the structures and energies of clusters. *Journal of Computational Chemistry*, 32(14):3075–3080, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Modesto-Costa:2015:WSE

[MCUJ15] Lucas Modesto-Costa, Elmar Uhl, and Itamar Borges Jr. Water solvent effects using continuum and discrete models: the nitromethane molecule, CH_3 NO_2. *Journal of Computational Chemistry*, 36(30):2260–2269, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2013:FES

[MCvdV13] Ning Ma, Ying-Hua Chung, and Arjan van der Vaart. Free energy simulation of helical transitions. *Journal of Computational Chemistry*, 34(8):640–645, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martins:2018:WQW

[MdOdQ18] João Paulo Ataide Martins, Marco Antônio Rougeth de Oliveira, and Mário Sérgio Oliveira de Queiroz. Web-4D-QSAR: a web-based application to generate 4D-QSAR descriptors. *Journal of Computational Chemistry*, 39(15): 917–924, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maupetit:2010:FML

[MDT10] Julien Maupetit, Philippe Derreumaux, and Pierre Tufféry. A fast method for large-scale De Novo peptide and miniprotein structure prediction. *Journal of Computational Chemistry*, 31 (4):726–738, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maintz:2013:APP

[MDTD13] Stefan Maintz, Volker L. Deringer, Andrei L. Tchougréeff, and Richard Dronskowski. Analytic projection from plane-wave and PAW wavefunctions and application to chemical-bonding analysis in solids. *Journal of Computational Chemistry*, 34 (29):2557–2567, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maintz:2016:SNU

[MDTD16] Stefan Maintz, Volker L. Deringer, Andrei L. Tchougréeff, and Richard Dronskowski. Software news and updates: LOBSTER: a tool to extract chemical bonding from plane-wave based DFT. *Journal of Computational Chemistry*, 37(11): 1030–1035, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miljacic:2010:RTA

[ME10] Lj. Miljacic and D. E. Ellis. Radial-template approach for accurate density representation in computational quantum theory. *Journal of Computational Chemistry*, 31(7):1486–1494, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morrison:2018:DBH

[MEH18] Adrian F. Morrison, Evgeny Epifanovsky, and John M. Herbert. Double-buffered, heterogeneous CPU + GPU integral digestion algorithm for single-excitation calculations involving a large number of excited states. *Journal of Computational Chemistry*, 39(26):2173–2182, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mezei:2010:SSF

[Mez10] Mihaly Mezei. Simulaid: a simulation facilitator and analysis program. *Journal of Computational Chemistry*, 31(14):2658–2668, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miao:2015:AMD

[MFEM15] Yinglong Miao, Ferran Feixas, Changsun Eun, and J. Andrew McCammon. Accelerated molecular dynamics simulations of protein folding. *Journal of Computational Chemistry*, 36(20): 1536–1549, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miao:2016:FAW

[MFEM16] Yinglong Miao, Ferran Feixas, Changsun Eun, and J. Andrew McCammon. The following articles were published in past issues of the *Journal of Computational Chemistry*: Accelerated molecular dynamics simulations of protein folding. *Journal of Computational Chemistry*, 37(6), March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Melia:2012:CSH

[MFM+12] Conchín Meliá, Silvia Ferrer, Vicent Moliner, Iñaki Tuñón, and Juan Bertrán. Computational study on hydrolysis of cefotaxime in gas phase and in aqueous solution. *Journal of Computational Chemistry*, 33(24):1948–1959, September 15,

2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Moreira:2010:PPD

[MFR10] Irina S. Moreira, Pedro A. Fernandes, and Maria J. Ramos. Protein–protein docking dealing with the unknown. *Journal of Computational Chemistry*, 31(2):317–342, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mollenhauer:2011:AQC

[MFR+11] Doreen Mollenhauer, Johannes Flob, Hans-Ulrich Reissig, Elena Voloshina, and Beate Paulus. Accurate quantum-chemical description of gold complexes with pyridine and its derivatives. *Journal of Computational Chemistry*, 32(9):1839–1845, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morao:2017:RAA

[MFR+17] Inaki Morao, Dmitri G. Fedorov, Roger Robinson, Michelle Southey, Andrea Townsend-Nicholson, Mike J. Bodkin, and Alexander Heifetz. Rapid and accurate assessment of GPCR–ligand interactions using the fragment molecular orbital-based density-functional tight-binding method. *Journal of Computational Chemistry*, 38(23):1987–1990, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Micera:2011:SOC

[MG11] Giovanni Micera and Eugenio Garribba. Is the spin-orbit coupling important in the prediction of the ^{51}V hyperfine coupling constants of $V^{IV}O^{2+}$ species? ORCA versus Gaussian performance and biological applications. *Journal of Computational Chemistry*, 32(13):2822–2835, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mollenhauer:2014:BPT

[MG14] Doreen Mollenhauer and Nicola Gaston. A balanced procedure for the treatment of cluster–ligand interactions on gold phosphine systems in catalysis. *Journal of Computational Chemistry*, 35(13):986–997, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marmitt:2015:DSI

[MG15] Sandro Marmitt and Paulo F. B. Gonçalves. A DFT study on the insertion of CO_2 into styrene oxide catalyzed by 1-butyl-3-methyl-Imidazolium bromide ionic liquid. *Journal of Computational Chemistry*, 36(17):1322–1333, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maschietto:2019:UDB

[MGCC19] Federica Maschietto, Juan Sanz García, Marco Campetella, and Ilaria Ciofini. Using density based indexes to characterize excited states evolution. *Journal of Computational Chemistry*, 40(4):650–656, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mulder:2016:SEO

[MGS+16] Joshua R. Mulder, Célia Fonseca Guerra, J. Chris Slootweg, Koop Lammertsma, and F. Matthias Bickelhaupt. Substituent effects on the optical properties of naphthalenediimides: a frontier orbital analysis across the periodic table. *Journal of Computational Chemistry*, 37(2):304–313, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mikulskis:2012:SAL

[MGWR12] Paulius Mikulskis, Samuel Genheden, Karin Wichmann, and Ulf Ryde. A semiempirical approach to ligand-binding affinities: Dependence on the Hamiltonian and corrections. *Journal of Computational Chemistry*, 33(12):1179–1189, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muta:2010:ASF

[MH10] Hajime Muta and Noriaki Hirayama. Alpha sphere filter method: Application of pseudomolecular descriptors in virtual screening of 2D chemical structures. *Journal of Computational Chemistry*, 31(11):2225–2232, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meng:2011:CSL

[MH11] Qingyong Meng and Ming-Bao Huang. A CAS study on S-loss and O-loss dissociation mechanisms of the SO_2^+ ion in the C, D, and E states. *Journal of Computational Chemistry*, 32(1):142–151, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meitei:2017:IIS

[MH17] Oinam Romesh Meitei and Andreas Heßelmann. Intramolecular interactions in sterically crowded hydrocarbon molecules. *Journal of Computational Chemistry*, 38(29):2500–2508, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maurer:2018:CFE

[MHO18] Manuela Maurer, Niels Hansen, and Chris Oostenbrink. Comparison of free-energy methods using a tripeptide-water model system. *Journal of Computational Chemistry*, 39(26):2226–2242, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Moin:2011:SDM

[MHRR11] Syed Tarique Moin, Thomas S. Hofer, Bernhard R. Randolf, and Bernd M. Rode. Structure and dynamics of methanol in water: a quantum mechanical charge field molecular dynamics study. *Journal of Computational Chemistry*, 32(5):886–892, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maeda:2018:SNU

[MHT+18] Satoshi Maeda, Yu Harabuchi, Makito Takagi, Kenichiro Saita, Kimichi Suzuki, Tomoya Ichino, Yosuke Sumiya, Kanami Sugiyama, and Yuriko Ono. Software news and updates: Implementation and performance of the artificial force induced reaction method in the GRRM17 program. *Journal of Computational Chemistry*, 39(4):233–251, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Minh:2018:PTI

[Min18] David D. L. Minh. Power transformations improve interpolation of grids for molecular mechanics interaction energies. *Journal of Computational Chemistry*, 39(19):1200–1207, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morishita:2013:FRF

[MIOM13] Tetsuya Morishita, Satoru G. Itoh, Hisashi Okumura, and Masuhiro Mikami. On-the-fly reconstruction of free-energy profiles using logarithmic mean-force dynamics. *Journal of Computational Chemistry*, 34(16):1375–1384, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muhammad:2015:HDH

[MIS+15] Shabbir Muhammad, Ahmad Irfan, Mohd Shkir, Aijaz R. Chaudhry, Abul Kalam, Salem AlFaify, Abdullah G. Al-Sehemi, A. E. Al-Salami, I. S. Yahia, Hong-Liang Xu, and Zhong-Min Su. How does hybrid bridging core modification enhance the nonlinear optical properties in donor-π-acceptor configuration? A case study of dinitrophenol derivatives. *Journal of Computational Chemistry*, 36(2):118–128, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitin:2013:PFM

[Mit13] Alexander V. Mitin. Polarization functions for the modified m6-31G basis sets for atoms Ga through Kr. *Journal of Computational Chemistry*, 34(23):2014–2019, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maingi:2012:DBT

[MJBM12] Vishal Maingi, Vaibhav Jain, Prasad V. Bharatam, and Prabal K. Maiti. Dendrimer building toolkit: Model building and characterization of various dendrimer architectures. *Journal of Computational Chemistry*, 33(25):1997–2011, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martin:2014:CAN

[MJC14] Hugh S. C. Martin, Shantenu Jha, and Peter V. Coveney. Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force. *Journal of Computational Chemistry*, 35(9): 692–702, April 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mones:2015:ABF

[MJG+15] Letif Mones, Andrew Jones, Andreas W. Götz, Teodoro Laino, Ross C. Walker, Ben Leimkuhler, Gábor Csányi, and Noam Bernstein. The adaptive buffered force QM/MM method in the CP2K and AMBER software packages. *Journal of Computational Chemistry*, 36(9):633–648, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marx:2014:CLH

[MJLV14a] Frans T. I. Marx, Johan H. L. Jordaan, Gerhard Lachmann, and Hermanus C. M. Vosloo. A comparison of low and high activity precatalysts: Do the calculated energy barriers during the self-metathesis reaction of 1-Octene correlate with the precatalyst metathesis activity? *Journal of Computational Chemistry*, 35(19):1464–1471, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marx:2014:MMS

[MJLV14b] Frans T. I. Marx, Johan H. L. Jordaan, Gerhard Lachmann, and Hermanus C. M. Vosloo. A Molecular modeling study of the changes of some steric properties of the precatalysts during the olefin metathesis reaction. *Journal of Computational Chemistry*, 35(19):1457–1463, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitoraj:2015:NWA

[MJM+15] Mariusz P. Mitoraj, Goran V. Janjić, Vesna B. Medaković, Dušan Ž. Veljković, Artur Michalak, Snežana D. Zarić, and Miloš K. Milčić. Nature of the water/aromatic parallel alignment interactions. *Journal of Computational Chemistry*, 36 (3):171–180, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mach:2011:GML

[MK11] Paul Mach and Patrice Koehl. Geometric measures of large biomolecules: Surface, volume, and pockets. *Journal of Computational Chemistry*, 32(14):3023–3038, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mach:2013:AMC

[MK13a] Paul Mach and Patrice Koehl. An analytical method for computing atomic contact areas in biomolecules. *Journal of Computational Chemistry*, 34(2):105–120, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malyszek:2013:AIP

[MK13b] Paweł Małyszek and Jacek Koput. Accurate Ab initio potential energy surface and vibration-rotation energy levels of hydrogen peroxide. *Journal of Computational Chemistry*, 34 (5):337–345, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McConnell:2017:IRC

[MK17] Sean McConnell and Johannes Kästner. Instanton rate constant calculations close to and above the crossover temperature. *Journal of Computational Chemistry*, 38(30):2570–2580, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McConnell:2019:IRC

[MK19] Sean R. McConnell and Johannes Kästner. Instanton rate constant calculations using interpolated potential energy surfaces in nonredundant, rotationally and translationally invariant coordinates. *Journal of Computational Chemistry*, 40(7): 866–874, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Moore:2013:HQP

[MKB+13] Benjamin L. Moore, Lawrence A. Kelley, James Barber, James W. Murray, and James T. MacDonald. High-quality protein backbone reconstruction from alpha carbons using Gaussian mixture models. *Journal of Computational Chemistry*, 34(22):1881–1889, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Makowski:2010:DEC

[MKGA10] Marcin Makowski, Jacek Korchowiec, Feng Long Gu, and Yuriko Aoki. Describing electron correlation effects in the framework of the elongation method — Elongation-MP2: Formalism, implementation and efficiency. *Journal of Computa-*

tional Chemistry, 31(8):1733–1740, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Merlot:2013:AEE

[MKH+13] Patrick Merlot, Thomas Kjærgaard, Trygve Helgaker, Roland Lindh, Francesco Aquilante, Simen Reine, and Thomas Bondo Pedersen. Attractive electron–electron interactions within robust local fitting approximations. *Journal of Computational Chemistry*, 34(17):1486–1496, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Middendorf:2015:SSB

[MKH15] Nils Middendorf, Katharina Krause, and Sebastian Höfener. Solvatochromic shifts of Br_2 and I_2 in water cages of type 5^{12}, 5^{12} 6^2, 5^{12} 6^3, and 5^{12} 6^4. *Journal of Computational Chemistry*, 36(11):853–860, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:2019:IFT

[MKK+19] Patrick Müller, Kristof Karhan, Matthias Krack, Uwe Gerstmann, Wolf Gero Schmidt, Matthias Bauer, and Thomas D. Kühne. Impact of finite-temperature and condensed-phase effects on theoretical X-ray absorption spectra of transition metal complexes. *Journal of Computational Chemistry*, 40 (5):712–716, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miyashita:2017:FFC

[MKM+17] Osamu Miyashita, Chigusa Kobayashi, Takaharu Mori, Yuji Sugita, and Florence Tama. Flexible fitting to cryo-EM density map using ensemble molecular dynamics simulations. *Journal of Computational Chemistry*, 38(16):1447–1461, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsui:2013:CSC

[MKO+13] Toru Matsui, Yasutaka Kitagawa, Mitsutaka Okumura, Yasuteru Shigeta, and Shigeyoshi Sakaki. Consistent scheme for computing standard hydrogen electrode and redox potentials. *Journal of Computational Chemistry*, 34(1):21–26, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marais:2012:ECM

[MKS+12] Patrick Marais, Julian Kenwood, Keegan Carruthers Smith, Michelle M. Kuttel, and James Gain. Efficient compression of molecular dynamics trajectory files. *Journal of Computational Chemistry*, 33(27):2131–2141, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mirzoev:2014:SIS

[ML14] Alexander Mirzoev and Alexander P. Lyubartsev. Systematic implicit solvent coarse graining of dimyristoylphosphatidylcholine lipids. *Journal of Computational Chemistry*, 35(16): 1208–1218, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohammed:2013:FOF

[MLC13] Ahmed A. K. Mohammed, Peter A. Limacher, and Benoît Champagne. Finding optimal finite field strengths allowing for a maximum of precision in the calculation of polarizabilities and hyperpolarizabilities. *Journal of Computational Chemistry*, 34(17):1497–1507, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mok:2011:FCS

[MLCD11] Daniel K. W. Mok, Edmond P. F. Lee, Foo-Tim Chau, and John M. Dyke. Franck–Condon simulation of the photoelectron spectrum of $AsCl_2$ and the photodetachment spectrum of AsCl employing UCCSD(T)-F12a potential energy functions: IE and EA of $AsCl_2$. *Journal of Computational Chemistry*, 32(8):1648–1660, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Macetti:2018:SDA

[MLG18] Giovanni Macetti, Leonardo Lo Presti, and Carlo Gatti. Spin density accuracy and distribution in azido Cu(II) complexes: a source function analysis. *Journal of Computational Chemistry*, 39(10):587–603, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Makarewicz:2016:NIF

[MLGB16] Emilia Makarewicz, Jan Lundell, Agnieszka J. Gordon, and Slawomir Berski. On the nature of interactions in the $F_2OXe{\cdots}NCCH_3$ complex: Is there the Xe(IV) — N bond?

Journal of Computational Chemistry, 37(20):1876–1886, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mermelstein:2018:FFG

[MLN+18] Daniel J. Mermelstein, Charles Lin, Gard Nelson, Rachael Kretsch, J. Andrew McCammon, and Ross C. Walker. Fast and flexible GPU accelerated binding free energy calculations within the amber molecular dynamics package. *Journal of Computational Chemistry*, 39(19):1354–1358, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2012:TIR

[MLQ+12] Nana Ma, Chunguang Liu, Yongqing Qiu, Shiling Sun, and Zhongmin Su. Theoretical investigation on redox-switchable second-order nonlinear optical responses of push–pull $Cp^*CoEt_2C_2B_4H_3$-expanded (metallo)porphyrins. *Journal of Computational Chemistry*, 33(2):211–219, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mo:2013:DSE

[MLY+13] Otilia Mó, Al Mokhtar Lamsabhi, Manuel Yáñez, Gavin S. Heverly-Coulson, and Russell J. Boyd. Dramatic substituent effects on the mechanisms of nucleophilic attack on Se—S bridges. *Journal of Computational Chemistry*, 34(29):2537–2547, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mei:2012:EPC

[MLZZ12] Ye Mei, Yong L. Li, Juan Zeng, and John Z. H. Zhang. Electrostatic polarization is critical for the strong binding in streptavidin-biotin system. *Journal of Computational Chemistry*, 33(15):1374–1382, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Massa:2018:QCP

[MM18] Lou Massa and Chérif F. Matta. Quantum crystallography: a perspective. *Journal of Computational Chemistry*, 39(17): 1021–1028, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maley:2019:IMS

[MM19] Steven M. Maley and Robert C. Mawhinney. Isothiirane: a molecular structure dilemma resolved. *Journal of Computational Chemistry*, 40(8):916–924, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Masetti:2017:DMM

[MMB+17] Matteo Masetti, Francesco Musiani, Mattia Bernetti, Federico Falchi, Andrea Cavalli, Stefano Ciurli, and Maurizio Recanatini. Development of a multisite model for Ni(II) ion in solution from thermodynamic and kinetic data. *Journal of Computational Chemistry*, 38(21):1834–1843, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malpathak:2019:AIU

[MMH19] Shreyas Malpathak, Xinyou Ma, and William L. Hase. Addressing an instability in unrestricted density functional theory direct dynamics simulations. *Journal of Computational Chemistry*, 40(8):933–936, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:2010:CCR

[MMJ10] Richard P. Muller, Ann E. Mattsson, and Curtis L. Janssen. Calculation of chemical reaction energies using the AM05 density functional. *Journal of Computational Chemistry*, 31(9): 1860–1863, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mamonov:2016:FGB

[MMM+16] Artem B. Mamonov, Mohammad Moghadasi, Hanieh Mirzaei, Shahrooz Zarbafian, Laurie E. Grove, Tanggis Bohnuud, Pirooz Vakili, Ioannis Ch. Paschalidis, Sandor Vajda, and Dima Kozakov. Focused grid-based resampling for protein docking and mapping. *Journal of Computational Chemistry*, 37(11):961–970, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maekawa:2016:RIO

[MMS16] Shintaro Maekawa, Krzysztof Moorthi, and Yasuteru Shigeta. Refractive indices of organo-metallic and -metalloid compounds: a long-range corrected DFT study. *Journal of Com-*

putational Chemistry, 37(32):2759–2769, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mirijanian:2014:DUA

[MMZW14] Dina T. Mirijanian, Ranjan V. Mannige, Ronald N. Zuckermann, and Stephen Whitelam. Development and use of an atomistic CHARMM-based forcefield for peptoid simulation. *Journal of Computational Chemistry*, 35(5):360–370, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez-Nunez:2015:AMF

[MN15] Emilio Martínez-Núñez. An automated method to find transition states using chemical dynamics simulations. *Journal of Computational Chemistry*, 36(4):222–234, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miyahara:2019:PSN

[MN19] Tomoo Miyahara and Hiroshi Nakatsuji. Photoelectron spectrum of NO_2^-: SAC-CI gradient study of vibrational–rotational structures. *Journal of Computational Chemistry*, 40(2):360–374, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Murata:2010:LSE

[MNNK10a] Katsumi Murata, Naoya Nagata, Isao Nakanishi, and Kazuo Kitaura. Ligand shape emerges in solvent dipole ordering region at ligand binding site of protein. *Journal of Computational Chemistry*, 31(4):791–796, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Murata:2010:SSD

[MNNK10b] Katsumi Murata, Naoya Nagata, Isao Nakanishi, and Kazuo Kitaura. SDOVS: a solvent dipole ordering-based method for virtual screening. *Journal of Computational Chemistry*, 31(15):2714–2722, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mori:2015:STB

[MO15] Yoshiharu Mori and Hisashi Okumura. Simulated tempering based on global balance or detailed balance conditions:

Suwa–Todo, heat bath, and Metropolis algorithms. *Journal of Computational Chemistry*, 36(31):2344–2349, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mori:2017:CCU

[MO17] Yoshiharu Mori and Yuko Okamoto. Conformational changes of ubiquitin under high pressure conditions: a pressure simulated tempering molecular dynamics study. *Journal of Computational Chemistry*, 38(15):1167–1173, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morpurgo:2015:DSC

[Mor15] Simone Morpurgo. A DFT study on Cu(I) coordination in Cu-ZSM-5: Effects of the functional choice and tuning of the ONIOM approach. *Journal of Computational Chemistry*, 36 (9):660–669, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morokuma:2019:F

[Mor19] Keiji Morokuma. Foreword. *Journal of Computational Chemistry*, 40(1):11–13, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mori:2012:ALS

[MOS12] Takaharu Mori, Fumiko Ogushi, and Yuji Sugita. Analysis of lipid surface area in protein–membrane systems combining Voronoi tessellation and Monte Carlo integration methods. *Journal of Computational Chemistry*, 33(3):286–293, January 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitra:2011:UCP

[MP11] Pralay Mitra and Debnath Pal. Using correlated parameters for improved ranking of protein–protein docking decoys. *Journal of Computational Chemistry*, 32(5):787–796, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marques:2013:DIG

[MP13] Jorge M. C. Marques and Francisco B. Pereira. A detailed investigation on the global minimum structures of mixed rare-gas clusters: Geometry, energetics, and site occupancy. *Journal of Computational Chemistry*, 34(6):505–517, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maxwell:2017:URR

[MP17a] Peter I. Maxwell and Paul L. A. Popelier. Unfavorable regions in the Ramachandran plot: Is it really steric hindrance? The interacting quantum atoms perspective. *Journal of Computational Chemistry*, 38(29):2459–2474, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Myers:2017:PLP

[MP17b] Christopher G. Myers and B. Montgomery Pettitt. Phage-like packing structures with mean field sequence dependence. *Journal of Computational Chemistry*, 38(15):1191–1197, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manzoor:2019:EPC

[MP19a] Taniya Manzoor and Altaf Hussain Pandith. Enhancing the photoresponse by CdSe-Dye-TiO_2-based multijunction systems for efficient dye-sensitized solar cells: a theoretical outlook. *Journal of Computational Chemistry*, 40(28):2444–2452, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mattsson:2019:DFT

[MP19b] Stefan Mattsson and Beate Paulus. Density functional theory calculations of structural, electronic, and magnetic properties of the 3 d metal trifluorides MF_3 (M = Ti–Ni) in the solid state. *Journal of Computational Chemistry*, 40(11): 1190–1197, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morgante:2019:ACC

[MP19c] Pierpaolo Morgante and Roberto Peverati. ACCDB: a collection of chemistry databases for broad computational purposes. *Journal of Computational Chemistry*, 40(6):839–848, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marques:2010:GCL

[MPA10] J. M. C. Marques, A. A. C. C. Pais, and P. E. Abreu. Generation and characterization of low-energy structures in atomic clusters. *Journal of Computational Chemistry*, 31(7):1495–1503, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marques:2012:UBB

[MPA12] J. M. C. Marques, A. A. C. C. Pais, and P. E. Abreu. On the use of big-bang method to generate low-energy structures of atomic clusters modeled with pair potentials of different ranges. *Journal of Computational Chemistry*, 33(4):442–452, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mukherjee:2011:FEG

[MPBJ11] Goutam Mukherjee, Niladri Patra, Poranjyoti Barua, and B. Jayaram. A fast empirical GAFF compatible partial atomic charge assignment scheme for modeling interactions of small molecules with biomolecular targets. *Journal of Computational Chemistry*, 32(5):893–907, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahler:2019:TMP

[MPJ+19] Andrew Mahler, Kassidy Panno, Benjamin G. Janesko, Salvador Moncho, and Edward N. Brothers. Tunable model promoters in DFT simulations of catalysts. *Journal of Computational Chemistry*, 40(19):1752–1757, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Minovski:2013:CBM

[MPNS13] Nikola Minovski, Andrej Perdih, Marjana Novic, and Tom Solmajer. Cluster-based molecular docking study for in silico identification of novel 6-fluoroquinolones as potential inhibitors against mycobacterium tuberculosis. *Journal of Computational Chemistry*, 34(9):790–801, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Michael:2017:SMN

[MPSA17] Eleni Michael, Savvas Polydorides, Thomas Simonson, and Georgios Archontis. Simple models for nonpolar solvation: Parameterization and testing. *Journal of Computational*

Chemistry, 38(29):2509–2519, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahanta:2011:ISP

[MPSG11] Subrata Mahanta, Bijan Kumar Paul, Rupashree Balia Singh, and Nikhil Guchhait. Inequivalence of substitution pairs in hydroxynaphthaldehyde: a theoretical measurement by intramolecular hydrogen bond strength, aromaticity, and excited-state intramolecular proton transfer reaction. *Journal of Computational Chemistry*, 32(1):1–14, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miriyala:2017:DNC

[MŘ17] Vijay Madhav Miriyala and Jan Řezáč. Description of non-covalent interactions in SCC-DFTB methods. *Journal of Computational Chemistry*, 38(10):688–697, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mandado:2014:AER

[MRB14] Marcos Mandado and Nicolás Ramos-Berdullas. Analyzing the electric response of molecular conductors using “electron deformation” orbitals and occupied-virtual electron transfer. *Journal of Computational Chemistry*, 35(17):1261–1269, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Macchi:2018:ETE

[MRC+18] Piero Macchi, Fabio Ragaini, Nicola Casati, Anna Krawczuk, and Angelo Sironi. Experimental and theoretical electron density of intermediates in palladium-phenanthroline catalyzed carbonylation of amines and reductive carbonylation of nitroarenes. *Journal of Computational Chemistry*, 39(10):581–586, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meisner:2011:KIE

[MRK11] Jan Meisner, Judith B. Rommel, and Johannes Kästner. Kinetic isotope effects calculated with the instanton method. *Journal of Computational Chemistry*, 32(16):3456–3463, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Margreitter:2017:UPC

[MRO17] Christian Margreitter, Maria M. Reif, and Chris Oostenbrink. Update on phosphate and charged post-translationally modified amino acid parameters in the GROMOS force field. *Journal of Computational Chemistry*, 38(10):714–720, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mayeno:2011:REA

[MRR11] Arthur N. Mayeno, Jonathan L. Robinson, and Brad Reisfeld. Rapid estimation of activation enthalpies for cytochrome-P450-mediated hydroxylations. *Journal of Computational Chemistry*, 32(4):639–657, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manz:2010:DRC

[MS10] Thomas A. Manz and David S. Sholl. A dimensionless reaction coordinate for quantifying the lateness of transition states. *Journal of Computational Chemistry*, 31(7):1528–1541, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miao:2011:RHB

[MS11] Chuang Miao and Ying Shi. Reconsideration on hydrogen bond strengthening or cleavage of photoexcited coumarin 102 in aqueous solvent: a DFT/TDDFT study. *Journal of Computational Chemistry*, 32(14):3058–3061, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Moura:2012:QMM

[MS12] Gustavo L. C. Moura and Alfredo M. Simas. Quantum molecular mechanics — a noniterative procedure for the fast ab initio calculation of closed shell systems. *Journal of Computational Chemistry*, 33(9):958–969, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martins:2013:CAC

[MS13] Silvia A. Martins and Sergio F. Sousa. Comparative assessment of computational methods for the determination of solvation free energies in alcohol-based molecules. *Journal of Computational Chemistry*, 34(15):1354–1362, June 5, 2013.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:2015:CSN

[MS15] Carsten Müller and Daniel Spångberg. Calculation of the stability of nonperiodic solids using classical force fields and the method of increments: N_2O as an example. *Journal of Computational Chemistry*, 36(18):1420–1427, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mignon:2016:CTS

[MS16] David Mignon and Thomas Simonson. Comparing three stochastic search algorithms for computational protein design: Monte Carlo, replica exchange Monte Carlo, and a multistart, steepest-descent heuristic. *Journal of Computational Chemistry*, 37(19):1781–1793, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahajan:2017:JBP

[MS17] Swapnil Mahajan and Yves-Henri Sanejouand. Jumping between protein conformers using normal modes. *Journal of Computational Chemistry*, 38(18):1622–1630, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mishra:2012:CPM

[MSÅK12] Sushil Kumar Mishra, Johan Sund, Johan Åqvist, and Jaroslav Koča. Computational prediction of monosaccharide binding free energies to lectins with linear interaction energy models. *Journal of Computational Chemistry*, 33(29):2340–2350, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matta:2016:BMR

[MSBF16] Chérif F. Matta, Seyed Abdolreza Sadjadi, Dale A. Braden, and Gernot Frenking. The barrier to the methyl rotation in cis-2-butene and its isomerization energy to trans-2-butene, revisited. *Journal of Computational Chemistry*, 37(1):143–154, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marsili:2010:OMD

[MSC+10] Simone Marsili, Giorgio Federico Signorini, Riccardo Chelli, Massimo Marchi, and Piero Procacci. ORAC: a molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. *Journal of Computational Chemistry*, 31(5):1106–1116, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malolepsza:2010:SAC

[MSK+10] Edyta Małolepsza, Birgit Strodel, Mey Khalili, Semen Trygubenko, Szilard N. Fejer, and David J. Wales. Symmetrization of the AMBER and CHARMM force fields. *Journal of Computational Chemistry*, 31(7):1402–1409, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [MSK+12].

Malolepsza:2012:ESA

[MSK+12] Edyta Małolepsza, Birgit Strodel, Mey Khalili, Semen Trygubenko, Szilard Fejer, Joanne M. Carr, and David J. Wales. Erratum: "Symmetrization of the AMBER and CHARMM force fields" [J. Comp. Chem. **31**, 1402]. *Journal of Computational Chemistry*, 33(27):2209, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [MSK+10].

Maciejczyk:2010:CGM

[MSLS10] Maciej Maciejczyk, Aleksandar Spasic, Adam Liwo, and Harold A. Scheraga. Coarse-grained model of nucleic acid bases. *Journal of Computational Chemistry*, 31(8):1644–1655, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mielczarek:2019:GPE

[MSPC19] Detlev Conrad Mielczarek, Chourouk Nait Saidi, Patrice Paricaud, and Laurent Catoire. Generalized Prediction of Enthalpies of Formation Using DLPNO-CCSD(T) Ab Initio Calculations for Molecules Containing the Elements H, C, N, O, F, S, Cl, Br. *Journal of Computational Chemistry*, 40(6):768–793, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mayne:2013:RPS

[MSS+13] Christopher G. Mayne, Jan Saam, Klaus Schulten, Emad Tajkhorshid, and James C. Gumbart. Rapid parameterization of small molecules using the force field toolkit. *Journal of Computational Chemistry*, 34(32):2757–2770, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mills:2017:SNU

[MSSP17] Matthew J. L. Mills, Kenneth L. Sale, Blake A. Simmons, and Paul L. A. Popelier. Software news and updates: Rhorix: an interface between quantum chemical topology and the 3D graphics program blender. *Journal of Computational Chemistry*, 38(29):2538–2552, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez:2016:TER

[MSV16] Juan Pablo Martínez, Miquel Solà, and Alexander A. Voityuk. Theoretical estimation of the rate of photoinduced charge transfer reactions in triphenylamine C_{60} donor–acceptor conjugate. *Journal of Computational Chemistry*, 37(15):1396–1405, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meier:2012:IGB

[MSvG12] Katharina Meier, Nathan Schmid, and Wilfred F. van Gunsteren. Interfacing the GROMOS (bio)molecular simulation software to quantum-chemical program packages. *Journal of Computational Chemistry*, 33(26):2108–2117, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mananghaya:2019:SAG

[MSY19] Michael R. Mananghaya, Gil N. Santos, and Dennis Yu. Solubility of aminotriethylene glycol functionalized single wall carbon nanotubes: a density functional based tight binding molecular dynamics study. *Journal of Computational Chemistry*, 40(8):952–958, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahajan:2019:MCG

[MT19a] Subhamoy Mahajan and Tian Tang. Martini coarse-grained model for polyethylenimine. *Journal of Computational Chemistry*, 40(3):607–618, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [MT20].

Matsuzaki:2019:ENF

[MT19b] Rei Matsuzaki and Kazuo Takatsuka. Electronic and nuclear flux analysis on nonadiabatic electron transfer reaction: a view from single-configuration adiabatic Born–Huang representation. *Journal of Computational Chemistry*, 40(1):148–163, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahajan:2020:EMC

[MT20] Subhamoy Mahajan and Tian Tang. Erratum: "Martini Coarse-Grained Model for Polyethylenimine" [J. Comput. Chem. 2019, **40**, 607–618, DOI: 10.1002/jcc.25747]. *Journal of Computational Chemistry*, 41(18):1730–1734, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [MT19a].

Maeda:2014:ETS

[MTM14] Satoshi Maeda, Tetsuya Taketsugu, and Keiji Morokuma. Exploring transition state structures for intramolecular pathways by the artificial force induced reaction method. *Journal of Computational Chemistry*, 35(2):166–173, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsumoto:2019:ACC

[MTS+19] Kentaro Matsumoto, Masayoshi Takayanagi, Yuichi Suzuki, Nobuaki Koga, and Masataka Nagaoka. Atomistic chemical computation of olefin polymerization reaction catalyzed by (pyridylamido)hafnium(IV) complex: Application of Red Moon simulation. *Journal of Computational Chemistry*, 40(2):421–429, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meier:2012:EVF

[MTvG12] Katharina Meier, Walter Thiel, and Wilfred F. van Gunsteren. On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations. *Journal of Computational Chemistry*, 33(4):363–378, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mena-Ulecia:2018:SAB

[MUGNVJ+18] Karel Mena-Ulecia, Fabian Gonzalez-Norambuena, Ariela Vergara-Jaque, Horacio Poblete, William Tiznado, and Julio Caballero. Study of the affinity between the protein kinase PKA and homoarginine-containing peptides derived from kemptide: Free energy perturbation (FEP) calculations. *Journal of Computational Chemistry*, 39(16):986–992, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2019:SEO

[MUN+19] Zhifeng Ma, Kasumi Ukaji, Naoki Nakatani, Hiroshi Fujii, and Masahiko Hada. Substitution effects on olefin epoxidation catalyzed by Oxoiron(IV) porphyrin π-cation radical complexes: a DFT study. *Journal of Computational Chemistry*, 40(19): 1780–1788, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohammadiarani:2017:IMP

[MV17] Hossein Mohammadiarani and Harish Vashisth. Insulin mimetic peptide S371 folds into a helical structure. *Journal of Computational Chemistry*, 38(15):1158–1166, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Myburgh:2018:CEC

[MvBD18] Dirkie Myburgh, Stuart von Berg, and Jan Dillen. A comparison of energetic criteria to probe the stabilizing interaction resulting from a bond path between congested atoms. *Journal of Computational Chemistry*, 39(27):2273–2282, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mohan:2010:CAN

[MVKS10] Neetha Mohan, Kunduchi P. Vijayalakshmi, Nobuaki Koga, and Cherumuttathu H. Suresh. Comparison of aromatic NH$\cdots\pi$, OH$\cdots\pi$, and CH$\cdots\pi$ interactions of alanine using MP2, CCSD, and DFT methods. *Journal of Computational Chemistry*, 31(16):2874–2882, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mo:2019:E

[MWC19] Yirong Mo, Wei Wu, and Zexing Cao. Editorial. *Journal of Computational Chemistry*, 40(9):965, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miao:2011:DFT

[MWJ+11] Yuan Miao, Xueye Wang, Xin Jin, Ling Yi, and Cuihuan Ren. Density functional theory study of a molecular allosteric switch for 2,2'-bipyridyl-3,3'-15-crown-5. *Journal of Computational Chemistry*, 32(3):406–415, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsuzaki:2017:CPD

[MY17a] Rei Matsuzaki and Satoshi Yabushita. Calculation of photoionization differential cross sections using complex Gauss-type orbitals. *Journal of Computational Chemistry*, 38(23): 2030–2040, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsuzaki:2017:OCS

[MY17b] Rei Matsuzaki and Satoshi Yabushita. Optimization of complex Slater-type functions with analytic derivative methods for describing photoionization differential cross sections. *Journal of Computational Chemistry*, 38(12):910–925, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitsuta:2018:ASM

[MYKO18] Yuki Mitsuta, Shusuke Yamanaka, Takashi Kawakami, and Mitsutaka Okumura. Automated Search of Minimum Free-Energy Path by Umbrella Integration. *Journal of Computational Chemistry*, 39(23):1913–1921, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maruyama:2014:MPI

[MYT$^+$14] Yutaka Maruyama, Norio Yoshida, Hiroto Tadano, Daisuke Takahashi, Mitsuhisa Sato, and Fumio Hirata. Massively parallel implementation of 3D-RISM calculation with volumetric 3D-FFT. *Journal of Computational Chemistry*, 35(18): 1347–1355, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsumoto:2018:SNU

[MYT18] Masakazu Matsumoto, Takuma Yagasaki, and Hideki Tanaka. Software news and updates: GenIce: Hydrogen-disordered ice generator. *Journal of Computational Chemistry*, 39(1):61–64, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mamonov:2011:RSA

[MZZ11] Artem B. Mamonov, Xin Zhang, and Daniel M. Zuckerman. Rapid sampling of all-atom peptides using a library-based polymer-growth approach. *Journal of Computational Chemistry*, 32(3):396–405, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nemoto:2015:ISN

[NASH15] Keisuke Nemoto, Minori Abe, Junji Seino, and Masahiko Hada. An ab initio study of nuclear volume effects for isotope fractionations using two-component relativistic methods. *Journal of Computational Chemistry*, 36(11):816–820, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nava:2018:IDM

[Nav18] M. Nava. Implementing dimer metadynamics using gromacs. *Journal of Computational Chemistry*, 39(25):2126–2132, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakata:2019:DNP

[NB19] Hiroya Nakata and Shandan Bai. Development of a new parameter optimization scheme for a reactive force field based on a machine learning approach. *Journal of Computational Chemistry*, 40(23):2000–2012, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neogi:2012:SSW

[NC12] Soumya Ganguly Neogi and Pinaki Chaudhury. Structure and spectroscopy of water-fluoride microclusters: a combined genetic algorithm and DFT-based study. *Journal of Computational Chemistry*, 33(6):629–639, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neogi:2013:SSA

[NC13] Soumya Ganguly Neogi and Pinaki Chaudhury. Structure and spectroscopic aspects of water-halide ion clusters: a study based on a conjunction of stochastic and quantum chemical methods. *Journal of Computational Chemistry*, 34(6):471–491, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neogi:2014:SSA

[NC14] Soumya Ganguly Neogi and Pinaki Chaudhury. Structural, spectroscopic aspects, and electronic properties of $(TiO_2)_n$ clusters: a study based on the use of natural algorithms in association with quantum chemical methods. *Journal of Computational Chemistry*, 35(1):51–61, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ninno:2018:RSG

[NCT18] Domenico Ninno, Giovanni Cantele, and Fabio Trani. Real-space grid representation of momentum and kinetic energy operators for electronic structure calculations. *Journal of Computational Chemistry*, 39(20):1406–1412, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nemeth:2010:CIC

[NCV10] Károly Németh, Matt Challacombe, and Michel Van Veenendaal. The choice of internal coordinates in complex chemical systems. *Journal of Computational Chemistry*, 31(10):2078–2086, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nikitin:2019:DNM

[ND19] Alexei Nikitin and Gianluca Del Frate. Development of nonbonded models for metal cations using the electronic continuum correction. *Journal of Computational Chemistry*, 40(28):

2464–2472, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Noel:2010:USI

[NDD+10] Yves Noel, Philippe D'arco, Raffaella Demichelis, Claudio M. Zicovich-Wilson, and Roberto Dovesi. On the use of symmetry in the ab initio quantum mechanical simulation of nanotubes and related materials. *Journal of Computational Chemistry*, 31(4):855–862, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nieto:2014:BNM

[NDG14] Carlos T. Nieto, David Díez, and Narciso M. Garrido. To be or not to be butterfly: New mechanistic insights in the Aza–Michael asymmetric addition of lithium (R)-N-benzyl-N-(α-methylbenzyl)amide. *Journal of Computational Chemistry*, 35(25):1846–1853, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neumann:2013:MDM

[NDLW13] Tobias Neumann, Denis Danilov, Christian Lennartz, and Wolfgang Wenzel. Modeling disordered morphologies in organic semiconductors. *Journal of Computational Chemistry*, 34(31):2716–2725, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neumann:2015:MMA

[NDW15] Tobias Neumann, Denis Danilov, and Wolfgang Wenzel. Multiparticle moves in acceptance rate optimized Monte Carlo. *Journal of Computational Chemistry*, 36(30):2236–2245, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishimoto:2017:TBE

[NF17] Yoshio Nishimoto and Dmitri G. Fedorov. Three-body expansion of the fragment molecular orbital method combined with density-functional tight-binding. *Journal of Computational Chemistry*, 38(7):406–418, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakata:2018:ASD

[NF18] Hiroya Nakata and Dmitri G. Fedorov. Analytic second derivatives for the efficient electrostatic embedding in the fragment molecular orbital method. *Journal of Computational Chemistry*, 39(25):2039–2050, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nicolini:2013:TQE

[NFG+13] Paolo Nicolini, Diego Frezzato, Cristina Gellini, Marco Bizzarri, and Riccardo Chelli. Toward quantitative estimates of binding affinities for protein–ligand systems involving large inhibitor compounds: a steered molecular dynamics simulation route. *Journal of Computational Chemistry*, 34(18): 1561–1576, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nozaki:2016:TSL

[NFI+16] Hiroo Nozaki, Yosuke Fujii, Kazuhide Ichikawa, Taku Watanabe, Yuichi Aihara, and Akitomo Tachibana. Theoretical study of lithium ionic conductors by electronic stress tensor density and electronic kinetic energy density. *Journal of Computational Chemistry*, 37(20):1924–1934, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nickerson:2013:CCW

[NFPD13] Stella Nickerson, Denzil S. Frost, Harrison Phelan, and Lenore L. Dai. Comparison of the capillary wave method and pressure tensor route for calculation of interfacial tension in molecular dynamics simulations. *Journal of Computational Chemistry*, 34(31):2707–2715, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Noy:2010:FPP

[NG10] Efrat Noy and Amiram Goldblum. Flexible protein-protein docking based on Best-First search algorithm. *Journal of Computational Chemistry*, 31(9):1929–1943, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Namsani:2017:IPS

[NGAS17] Sadanandam Namsani, Bhasker Gahtori, Sushil Auluck, and Jayant K. Singh. An interaction potential to study the thermal structure evolution of a thermoelectric material: β-Cu_2Se. *Journal of Computational Chemistry*, 38(25):2161–

2170, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakatani:2019:CLA

[NH19] Naoki Nakatani and Masahiko Hada. Can large active-space CASSCF calculation make sense to the reaction analysis of iron complex? A benchmark study of methane oxidation reaction by FeO^+. *Journal of Computational Chemistry*, 40(2): 414–420, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Najeh:2010:ETS

[NHF+10] Rekik Najeh, Ghalla Houcine, Henryk T. Flakus, Magdalena Jablonska, and Oujia Brahim. Experimental and theoretical study of the polarized infrared spectra of the hydrogen bond in 3-thiophenic acid crystal. *Journal of Computational Chemistry*, 31(3):463–475, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nowosielski:2013:MTC

[NHK+13] Marcin Nowosielski, Marcin Hoffmann, Aneta Kuron, Małgorzata Korycka-Machala, and Jarosław Dziadek. The MM2QM tool for combining docking, molecular dynamics, molecular mechanics, and quantum mechanics. *Journal of Computational Chemistry*, 34(9):750–756, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ngo:2016:FAD

[NHN16] Son Tung Ngo, Huynh Minh Hung, and Minh Tho Nguyen. Fast and accurate determination of the relative binding affinities of small compounds to HIV-1 protease using non-equilibrium work. *Journal of Computational Chemistry*, 37 (31):2734–2742, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nozaki:2015:EST

[NIIT15] Hiroo Nozaki, Yuji Ikeda, Kazuhide Ichikawa, and Akitomo Tachibana. Electronic stress tensor analysis of molecules in gas phase of CVD process for GeSbTe alloy. *Journal of Computational Chemistry*, 36(16):1240–1251, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nizovtsev:2013:ACH

[Niz13] Anton S. Nizovtsev. Activation of C–H bond in methane by Pd atom from the bonding evolution theory perspective. *Journal of Computational Chemistry*, 34(22):1917–1924, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2018:ARR

[NJR18] Minh Khoa Nguyen, Léonard Jaillet, and Stéphane Redon. ART-RRT: As-rigid-as-possible exploration of ligand unbinding pathways. *Journal of Computational Chemistry*, 39(11): 665–678, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Niu:2010:RMM

[NJX+10] Cui-Yu Niu, Jiao Jiao, Bin Xing, Gui-Chang Wang, and Xian-He Bu. Reaction mechanism of methanol decomposition on Pt-based model catalysts: a theoretical study. *Journal of Computational Chemistry*, 31(10):2023–2037, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakamura:2019:PHA

[NK19] Taiji Nakamura and Takako Kudo. The planarity of heteroatom analogues of benzene: Energy component analysis and the planarization of hexasilabenzene. *Journal of Computational Chemistry*, 40(3):581–590, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nikolaienko:2018:EBE

[NKD18] Tymofii Yu. Nikolaienko, Eugene S. Kryachko, and Grygoriy A. Dolgonos. On the Existence of He–He bond in the endohedral fullerene He_2 @C_{60}. *Journal of Computational Chemistry*, 39(18):1090–1102, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nath:2016:SNU

[NKJ16] Shilpa R. Nath, Sudheer S. Kurup, and Kaustubh A. Joshi. Software news and updates: PyGlobal: a toolkit for automated compilation of DFT-based descriptors. *Journal of Computational Chemistry*, 37(16):1505–1510, June 15, 2016.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ni:2019:FOI

[NLL19] Zhigang Ni, Wei Li, and Shuhua Li. Fully optimized implementation of the cluster-in-molecule local correlation approach for electron correlation calculations of large systems. *Journal of Computational Chemistry*, 40(10):1130–1140, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Narth:2016:SIS

[NLP+16] Christophe Narth, Louis Lagardère, Étienne Polack, Nohad Gresh, Qiantao Wang, David R. Bell, Joshua A. Rackers, Jay W. Ponder, Pengyu Y. Ren, and Jean-Philip Piquemal. Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. *Journal of Computational Chemistry*, 37(5):494–506, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nivedha:2014:ILC

[NMF+14] Anita K. Nivedha, Spandana Makeneni, Bethany Lachele Foley, Matthew B. Tessier, and Robert J. Woods. Importance of ligand conformational energies in carbohydrate docking: Sorting the wheat from the chaff. *Journal of Computational Chemistry*, 35(7):526–539, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2019:HGM

[NMH19] Hieu Thanh Nguyen, Tam Van-Thanh Mai, and Lam Kim Huynh. mHDFS–HoF: a generalized multilevel homodesmotic fragment-separation reaction based program for heat-of-formation calculation for acyclic hydrocarbons. *Journal of Computational Chemistry*, 40(13):1360–1373, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ng:2013:RCC

[NMLD13] Maggie Ng, Daniel K. W. Mok, Edmond P. F. Lee, and John M. Dyke. Rate coefficients of the CF_3CHFCF_3 + H

$\rightarrow CF_3CFCF_3 + H_2$ reaction at different temperatures calculated by transition state theory with ab initio and DFT reaction paths. *Journal of Computational Chemistry*, 34(7): 545–557, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishimura:2018:PIE

[NN18] Yoshifumi Nishimura and Hiromi Nakai. Parallel implementation of efficient charge–charge interaction evaluation scheme in periodic divide-and-conquer density-functional tight-binding calculations. *Journal of Computational Chemistry*, 39(2):105–116, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishimura:2019:DCD

[NN19] Yoshifumi Nishimura and Hiromi Nakai. D cdftbmd: Divide-and-conquer density functional tight-binding program for huge-system quantum mechanical molecular dynamics simulations. *Journal of Computational Chemistry*, 40(15):1538–1549, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishizawa:2016:TPA

[NNK+16] Hiroaki Nishizawa, Yoshifumi Nishimura, Masato Kobayashi, Stephan Irle, and Hiromi Nakai. Three pillars for achieving quantum mechanical molecular dynamics simulations of huge systems: Divide-and-conquer, density-functional tight-binding, and massively parallel computation. *Journal of Computational Chemistry*, 37(21):1983–1992, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Namsani:2015:IPM

[NNS15] Sadanandam Namsani, Nisanth N. Nair, and Jayant K. Singh. Interaction potential models for bulk Zns, Zns nanoparticle, and Zns nanoparticle-PMMA from first principles. *Journal of Computational Chemistry*, 36(15):1176–1186, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakano:2019:QME

[NNT+19] Masayoshi Nakano, Takanori Nagami, Takayoshi Tonami, Kenji Okada, Soichi Ito, Ryohei Kishi, Yasutaka Kitagawa, and Takashi Kubo. Quantum master equation approach to singlet fission dynamics in pentacene linear aggregate models: Size dependences of excitonic coupling effects. *Journal of Computational Chemistry*, 40(1):89–104, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishizawa:2016:RQM

[NO16] Hiroaki Nishizawa and Hisashi Okumura. Rapid QM/MM approach for biomolecular systems under periodic boundary conditions: Combination of the density-functional tight-binding theory and particle mesh Ewald method. *Journal of Computational Chemistry*, 37(31):2701–2711, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Norby:2016:MME

[NOKJ16] Morten S. Nørby, Jógvan Magnus Haugaard Olsen, Jacob Kongsted, and Hans Jørgen Aagard Jensen. Multipole moments for embedding potentials: Exploring different atomic allocation algorithms. *Journal of Computational Chemistry*, 37(20):1887–1896, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ng:2017:RFT

[NPG17] Cathy Ng, Padmavathy Nandha Premnath, and Olgun Guvench. Rigidity and flexibility in the tetrasaccharide linker of proteoglycans from atomic-resolution molecular simulation. *Journal of Computational Chemistry*, 38(16):1438–1446, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Narsaria:2018:RDN

[NPG+18] Ayush K. Narsaria, Jordi Poater, Célia Fonseca Guerra, Andreas W. Ehlers, Koop Lammertsma, and F. Matthias Bickelhaupt. Rational design of near-infrared absorbing organic dyes: Controlling the HOMO–LUMO gap using quantitative molecular orbital theory. *Journal of Computational Chemistry*, 39(32):2690–2696, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nunes:2013:NAP

[NPP13] Sandra C. C. Nunes, P. Pinto, and A. A. C. C. Pais. Nonrandom adsorption of polyelectrolyte chains on finite regularly charged surfaces. *Journal of Computational Chemistry*, 34(14):1198–1209, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nagai:2016:UMS

[NPTS16] Tetsuro Nagai, George A. Pantelopulos, Takuya Takahashi, and John E. Straub. On the use of mass scaling for stable and efficient simulated tempering with molecular dynamics. *Journal of Computational Chemistry*, 37(21):2017–2028, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nandi:2019:DMC

[NQB19] Apurba Nandi, Chen Qu, and Joel M. Bowman. Diffusion Monte Carlo Calculations of Zero-Point Energies of Methanol and Deuterated Methanol. *Journal of Computational Chemistry*, 40(2):328–332, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nekouzadeh:2011:TRL

[NR11] Ali Nekouzadeh and Yoram Rudy. Three-residue loop closure in proteins: a new kinematic method reveals a locus of connected loop conformations. *Journal of Computational Chemistry*, 32(12):2515–2525, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nagar:2010:MDI

[NS10] Shuchi Nagar and Achintya Saha. Modeling of diarylalkyl-imidazole and diarylalkyl-triazole derivatives as potent aromatase inhibitors for treatment of hormone-dependent cancer. *Journal of Computational Chemistry*, 31(12):2342–2353, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ng:2011:PPP

[NS11] Albert H. Ng and Christopher D. Snow. Polarizable protein packing. *Journal of Computational Chemistry*, 32(7):1334–1344, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nozaki:2017:CDA

[NS17] Daijiro Nozaki and Wolf Gero Schmidt. Current density analysis of electron transport through molecular wires in open quantum systems. *Journal of Computational Chemistry*, 38 (19):1685–1692, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2018:HDF

[NS18] Thao P. Nguyen and Ji Hoon Shim. Hybrid density functional study on the electronic structures and properties of P3HT-PbS and P3HT-CdS hybrid interface for photovoltaic applications. *Journal of Computational Chemistry*, 39(24): 1990–1999, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Na:2018:TIN

[NSK18] Sehee Na, Thomas Steinbrecher, and Thorsten Koslowski. Thermodynamic integration network approach to ion transport through protein channels: Perspectives and limits. *Journal of Computational Chemistry*, 39(30):2539–2550, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nhat:2019:CTI

[NSN19] Pham Vu Nhat, Nguyen Thanh Si, and Minh Tho Nguyen. Comment on “Theoretical Investigations on Geometrical and Electronic Structures of Silver Clusters”. *Journal of Computational Chemistry*, 40(22):1990–1993, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [Tsu19].

Nantasenamat:2014:IOS

[NSO+14] Chanin Nantasenamat, Saw Simeon, Wiwat Owasirikul, Napat Songtawee, Maris Lapins, Virapong Prachayasittikul, and Jarl E. S. Wikberg. Illuminating the origins of spectral properties of green fluorescent proteins via proteochemometric and molecular modeling. *Journal of Computational Chemistry*, 35 (27):1951–1966, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nunes:2015:CPC

[NSP15] Sandra C. C. Nunes, Marie Skepö, and Alberto A. C. C. Pais. Confined polyelectrolytes: the complexity of a simple system. *Journal of Computational Chemistry*, 36(21):1579–1586, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Negami:2014:CGM

[NST14] Tatsuki Negami, Kentaro Shimizu, and Tohru Terada. Coarse-grained molecular dynamics simulations of protein–ligand binding. *Journal of Computational Chemistry*, 35(25): 1835–1845, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nozawa:2015:CAP

[NTNY15] Takuma Nozawa, Kazuaki Z. Takahashi, Tetsu Narumi, and Kenji Yasuoka. Comparison of the accuracy of periodic reaction field methods in molecular dynamics simulations of a model liquid crystal system. *Journal of Computational Chemistry*, 36(32):2406–2411, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2017:ISA

[NW17] Duc D. Nguyen and Guo-Wei Wei. The impact of surface area, volume, curvature, and Lennard-Jones potential to solvation modeling. *Journal of Computational Chemistry*, 38(1): 24–36, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2017:ARR

[NWW17] Duc D. Nguyen, Bao Wang, and Guo-Wei Wei. Accurate, robust, and reliable calculations of Poisson–Boltzmann binding energies. *Journal of Computational Chemistry*, 38(13): 941–948, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakano:2017:CIH

[NYH+17] Masahiko Nakano, Takeshi Yoshikawa, So Hirata, Junji Seino, and Hiromi Nakai. Computerized implementation of higher-order electron-correlation methods and their linear-scaling divide-and-conquer extensions. *Journal of Computational*

Chemistry, 38(29):2520–2527, November 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakai:2017:EPS

[NYN17] Hiromi Nakai, Takeshi Yoshikawa, and Yutaro Nonaka. Efficient pole-search algorithm for dynamic polarizability: Toward alternative excited-state calculation for large systems. *Journal of Computational Chemistry*, 38(1):7–14, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2018:UFF

[NZM18] Trung Hai Nguyen, Huan-Xiang Zhou, and David D. L. Minh. Using the Fast Fourier Transform in binding free energy calculations. *Journal of Computational Chemistry*, 39(11):621–636, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Okoshi:2015:REC

[OAN15a] Masaki Okoshi, Teruo Atsumi, and Hiromi Nakai. Revisiting the extrapolation of correlation energies to complete basis set limit. *Journal of Computational Chemistry*, 36(14):1075–1082, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ootani:2015:TIE

[OAN15b] Yusuke Ootani, Yoshinobu Akinaga, and Takahito Nakajima. Theoretical investigation of enantioselectivity of cage-like supramolecular assembly: the insights into the shape complementarity and host–guest interaction. *Journal of Computational Chemistry*, 36(7):459–466, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oehme:2012:EAC

[OBW12] Daniel P. Oehme, Robert T. C. Brownlee, and David J. D. Wilson. Effect of atomic charge, solvation, entropy, and ligand protonation state on MM-PB(GB)SA binding energies of HIV protease. *Journal of Computational Chemistry*, 33(32):2566–2580, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ozkanlar:2014:SNU

[OC14] Abdullah Ozkanlar and Aurora E. Clark. Software news and updates: ChemNetworks: a complex network analysis tool for chemical systems. *Journal of Computational Chemistry*, 35 (6):495–505, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ojha:2019:VES

[OC19] Deepak Ojha and Amalendu Chandra. Vibrational echo spectroscopy of aqueous sodium bromide solutions from first principles simulations. *Journal of Computational Chemistry*, 40 (24):2086–2095, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olson:2011:CBS

[OCL11] Mark A. Olson, Sidhartha Chaudhury, and Michael S. Lee. Comparison between self-guided Langevin dynamics and molecular dynamics simulations for structure refinement of protein loop conformations. *Journal of Computational Chemistry*, 32(14):3014–3022, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ortega-Carrasco:2014:APL

[OCLM14] Elisabeth Ortega-Carrasco, Agusti Lledós, and Jean-Didier Maréchal. Assessing protein–ligand docking for the binding of organometallic compounds to proteins. *Journal of Computational Chemistry*, 35(3):192–198, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ou:2015:FEC

[OCW+15] Shu-Ching Ou, Di Cui, Matthew Wezowicz, Michela Taufer, and Sandeep Patel. Free energetics of carbon nanotube association in aqueous inorganic NaI salt solutions: Temperature effects using all-atom molecular dynamics simulations. *Journal of Computational Chemistry*, 36(16):1196–1212, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Odinokov:2018:PAD

[ODB18] Alexey V. Odinokov, Nikita O. Dubinets, and Alexander A. Bagaturyants. pyEFP: Automatic decomposition of the complex molecular systems into rigid polarizable fragments. *Jour-*

nal of Computational Chemistry, 39(13):807–814, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Okumura:2010:CPL

[OGL10] Hisashi Okumura, Emilio Gallicchio, and Ronald M. Levy. Conformational populations of ligand-sized molecules by replica exchange molecular dynamics and temperature reweighting. *Journal of Computational Chemistry*, 31(7): 1357–1367, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohyama:2011:SIB

[OHNK11] Tatsuya Ohyama, Masato Hayakawa, Shin Nishikawa, and Noriyuki Kurita. Specific interactions between lactose repressor protein and DNA affected by ligand binding: Ab initio molecular orbital calculations. *Journal of Computational Chemistry*, 32(8):1661–1670, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oliver:2017:SSI

[OHPR17] Antoni Oliver, Christopher A. Hunter, Rafel Prohens, and Josep L. Rosselló. A surface site interaction point methodology for macromolecules and huge molecular databases. *Journal of Computational Chemistry*, 38(7):419–426, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oliver:2018:IMC

[OHPR18] Antoni Oliver, Christopher A. Hunter, Rafel Prohens, and Josep Lluis Rosselló. An improved methodology to compute surface site interaction points using high density molecular electrostatic potential surfaces. *Journal of Computational Chemistry*, 39(28):2371–2377, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohta:2016:PMB

[Oht16] Y. Ohta. Possible mechanism of BN fullerene formation from a boron cluster: Density-functional tight-binding molecular dynamics simulations. *Journal of Computational Chemistry*, 37(10):886–895, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oshima:2016:HEH

[OK16] Hiraku Oshima and Masahiro Kinoshita. A highly efficient hybrid method for calculating the hydration free energy of a protein. *Journal of Computational Chemistry*, 37(8):712–723, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohno:2017:GEI

[OKIS17] Koichi Ohno, Naoki Kishimoto, Takeaki Iwamoto, and Hiroko Satoh. Global exploration of isomers and isomerization channels on the quantum chemical potential energy surface of H_3CNO_3. *Journal of Computational Chemistry*, 38(10): 669–687, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohno:2018:QCE

[OKY18] Koichi Ohno, Yoshitomo Kodaya, and Hideo Yamakado. Quantum chemical exploration of formaldehyde clusters $(H_2CO)_n$ (n = 2–4). *Journal of Computational Chemistry*, 39(20):1498–1507, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olson:2013:ARE

[OL13] Mark A. Olson and Michael S. Lee. Application of replica exchange umbrella sampling to protein structure refinement of nontemplate models. *Journal of Computational Chemistry*, 34(20):1785–1793, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orimoto:2015:EME

[OLA15] Yuuichi Orimoto, Kai Liu, and Yuriko Aoki. Elongation method for electronic structure calculations of random DNA sequences. *Journal of Computational Chemistry*, 36(28):2103–2113, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oliveira:2019:BCS

[OLPB19] Daniel Vilela Oliveira, Joachim Laun, Michael F. Peintinger, and Thomas Bredow. BSSE-correction scheme for consistent Gaussian basis sets of double- and triple-zeta valence with polarization quality for solid-state calculations. *Journal of Computational Chemistry*, 40(27):2364–2376, October 15, 2019.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olson:2017:MIF

[OLY17] Mark A. Olson, Michael S. Lee, and In-Chul Yeh. Membrane insertion of fusion peptides from Ebola and Marburg viruses studied by replica-exchange molecular dynamics simulations. *Journal of Computational Chemistry*, 38(16):1342–1352, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otero:2012:CRF

[OM12] Nicolás Otero and Marcos Mandado. Chemical reactivity in the framework of pair density functional theories. *Journal of Computational Chemistry*, 33(13):1240–1251, May 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Osman:2016:RPS

[OME16] Roman Osman, Mihaly Mezei, and Stanislav Engel. The role of protein "stability patches" in molecular recognition: a case study of the human growth hormone-receptor complex. *Journal of Computational Chemistry*, 37(10):913–919, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Okoshi:2014:ASC

[ON14] Masaki Okoshi and Hiromi Nakai. Acceleration of self-consistent field convergence in ab initio molecular dynamics simulation with multiconfigurational wave function. *Journal of Computational Chemistry*, 35(20):1473–1480, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ortega:2016:CEN

[ONTTL16] Daniela E. Ortega, Quynh Nhu N. Nguyen, Dean J. Tantillo, and Alejandro Toro-Labbé. The catalytic effect of the NH_3 base on the chemical events in the caryolene-forming carbocation cascade. *Journal of Computational Chemistry*, 37(12):1068–1081, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ozawa:2011:ICH

[OOK11] Tomonaga Ozawa, Kosuke Okazaki, and Kazuo Kitaura. Importance of CH/π hydrogen bonds in recognition of the core motif in proline-recognition domains: An ab initio fragment molecular orbital study. *Journal of Computational Chemistry*, 32(13):2774–2782, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otsuka:2015:AAB

[OOT15] Takao Otsuka, Noriaki Okimoto, and Makoto Taiji. Assessment and acceleration of binding energy calculations for protein-ligand complexes by the fragment molecular orbital method. *Journal of Computational Chemistry*, 36(30):2209–2218, November 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orlando:2012:SNU

[OPB$^+$12] Roberto Orlando, Massimo Delle Piane, Ian J. Bush, Piero Ugliengo, Matteo Ferrabone, and Roberto Dovesi. Software news and updates: a new massively parallel version of CRYSTAL for large systems on high performance computing architectures. *Journal of Computational Chemistry*, 33(28):2276–2284, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Opletal:2017:RMC

[OPBR17] George Opletal, Timothy C. Petersen, Amanda S. Barnard, and Salvy P. Russo. On reverse Monte Carlo constraints and model reproduction. *Journal of Computational Chemistry*, 38 (17):1547–1551, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olah:2016:IGC

[OPR16] George A. Olah, G. K. Surya Prakash, and Golam Rasul. Ab initio /GIAO-CCSD(T)^{13} C NMR study of the rearrangement and dynamic aspects of rapidly equilibrating tertiary carbocations, $C_6H_{13}^+$ and $C_7H_{15}^+$. *Journal of Computational Chemistry*, 37(1):70–77, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Omar:2011:EOD

[ORZ11] Nasr Y. M. Omar, Noorsaadah A. Rahman, and Sharifuddin Md Zain. Enantioselective organocatalytic Diels–Alder reactions: a density functional theory and kinetic isotope effects study. *Journal of Computational Chemistry*, 32(9):1813–1823, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orimoto:2019:ESC

[OSA19] Yuuichi Orimoto, Satoru Shirane, and Yuriko Aoki. Extent of structural change during the reaction and its relationship to isoselectivity in polypropylene polymerization with ansa-zirconocene/borate catalyst: a computational study. *Journal of Computational Chemistry*, 40(30):2622–2635, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orthaber:2012:OVS

[OSF12] Andreas Orthaber, Alexander F. Sax, and Kevin A. Francesconi. Oxygen versus sulfur: Structure and reactivity of substituted arsine oxides and arsine sulfides. *Journal of Computational Chemistry*, 33(1):112–117, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orenha:2017:HCM

[OSHG17] Renato Pereira Orenha, Régis Tadeu Santiago, Roberto Luiz Andrade Haiduke, and Sérgio Emanuel Galembeck. How computational methods and relativistic effects influence the study of chemical reactions involving Ru–NO complexes? *Journal of Computational Chemistry*, 38(12):883–891, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohno:2019:ECA

[OSI+19] Koichi Ohno, Hiroko Satoh, Takeaki Iwamoto, Hiroaki Tokoyama, and Hideo Yamakado. Exploration of Carbon Allotropes with Four-membered Ring Structures on Quantum Chemical Potential Energy Surfaces. *Journal of Computational Chemistry*, 40(1):14–28, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olsson:2016:CLB

[OSR16] Martin A. Olsson, Pär Söderhjelm, and Ulf Ryde. Converging ligand-binding free energies obtained with free-energy perturbations at the quantum mechanical level. *Journal of Computational Chemistry*, 37(17):1589–1600, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oncak:2010:TSM

[OSS10] Milan Ončák, Detlef Schröder, and Petr Slavíček. Theoretical study of the microhydration of mononuclear and dinuclear uranium(VI) species derived from solvolysis of uranyl nitrate in water. *Journal of Computational Chemistry*, 31(12):2294–2306, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ootani:2012:IMD

[OT12] Yusuke Ootani and Tetsuya Taketsugu. Ab initio molecular dynamics approach to tunneling splitting in polyatomic molecules. *Journal of Computational Chemistry*, 33(1):60–65, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Olechnovic:2014:SNU

[OV14] Kliment Olechnovič and Česlovas Venclovas. Software news and updates: Voronota: a fast and reliable tool for computing the vertices of the Voronoi diagram of atomic balls. *Journal of Computational Chemistry*, 35(8):672–681, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otero:2015:HBI

[OVPK15] Nicolás Otero, Christian Van Alsenoy, Claude Pouchan, and Panaghiotis Karamanis. Hirshfeld-based intrinsic polarizability density representations as a tool to analyze molecular polarizability. *Journal of Computational Chemistry*, 36(24): 1831–1843, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Opron:2016:FRI

[OXBW16] Kristopher Opron, Kelin Xia, Zach Burton, and Guo-Wei Wei. Flexibility–rigidity index for protein–nucleic acid flexibility and fluctuation analysis. *Journal of Computational Chemistry*, 37(14):1283–1295, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Okamoto:2011:MIA

[OYK+11] Takuya Okamoto, Kenta Yamada, Yoshiyuki Koyano, Toshio Asada, Nobuaki Koga, and Masataka Nagaoka. A minimal implementation of the AMBER–GAUSSIAN interface for ab initio QM/MM-MD simulation. *Journal of Computational Chemistry*, 32(5):932–942, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [RSR+12].

Ostermeir:2014:HRE

[OZ14] Katja Ostermeir and Martin Zacharias. Hamiltonian replica-exchange simulations with adaptive biasing of peptide backbone and side chain dihedral angles. *Journal of Computational Chemistry*, 35(2):150–158, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ouk:2012:TST

[OZLSBH12] Chanda-Malis Ouk, Natalia Zvereva-Loëte, Yohann Scribano, and Béatrice Bussery-Honvault. Transition state theory thermal rate constants and RRKM-based branching ratios for the $N(^2D)$ + CH_4 reaction based on multi-state and multi-reference ab initio calculations of interest for the Titan's chemistry. *Journal of Computational Chemistry*, 33(28):2211–2224, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ouyang:2013:SNU

[OZS+13] Xuchang Ouyang, Shuo Zhou, Chinh Tran To Su, Zemei Ge, Runtao Li, and Chee Keong Kwoh. Software news and updates: CovalentDock: Automated covalent docking with parameterized covalent linkage energy estimation and molecular geometry constraints. *Journal of Computational Chemistry*, 34(4):326–336, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Partovi-Azar:2015:EFC

[PAK15] Pouya Partovi-Azar and Thomas D. Kühne. Efficient "on-the-fly" calculation of Raman spectra from ab-initio molecular dynamics: Application to hydrophobic/hydrophilic solutes in bulk water. *Journal of Computational Chemistry*, 36 (29):2188–2192, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Partovi-Azar:2017:TDD

[PAK17] Pouya Partovi-Azar and Payam Kaghazchi. Time-dependent density functional theory study on direction-dependent electron and hole transfer processes in molecular systems. *Journal of Computational Chemistry*, 38(10):698–703, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pasalic:2010:TSH

[PAT+10] Hasan Pašalić, Adélia J. A. Aquino, Daniel Tunega, Georg Haberhauer, Martin H. Gerzabek, Herbert C. Georg, Tatiane F. Moraes, Kaline Coutinho, Sylvio Canuto, and Hans Lischka. Thermodynamic stability of hydrogen-bonded systems in polar and nonpolar environments. *Journal of Computational Chemistry*, 31(10):2046–2055, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Peintinger:2014:CCM

[PB14] Michael F. Peintinger and Thomas Bredow. The cyclic cluster model at Hartree–Fock level. *Journal of Computational Chemistry*, 35(11):839–846, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pietropaolo:2011:CBM

[PBBP11] Adriana Pietropaolo, Davide Branduardi, Massimiliano Bonomi, and Michele Parrinello. A chirality-based metrics for free-energy calculations in biomolecular systems. *Journal of Computational Chemistry*, 32(12):2627–2637, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Perilla:2011:CET

[PBDW11] Juan R. Perilla, Oliver Beckstein, Elizabeth J. Denning, and Thomas B. Woolf. Computing ensembles of transitions from stable states: Dynamic importance sampling. *Journal of Computational Chemistry*, 32(2):196–209, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Porsev:2016:TDS

[PBE16] Vitaly V. Porsev, Andrei V. Bandura, and Robert A. Evarestov. Temperature dependence of strain energy and thermodynamic properties of V_2O_5-based single-walled nanotubes: Zone-folding approach. *Journal of Computational Chemistry*, 37(16):1442–1450, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pracht:2017:AEQ

[PBG17] Philipp Pracht, Christoph Alexander Bauer, and Stefan Grimme. Automated and efficient quantum chemical determination and energetic ranking of molecular protonation sites. *Journal of Computational Chemistry*, 38(30):2618–2631, November 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Palma:2012:CBA

[PBLdS12] P. Nuno Palma, Maria João Bonifácio, Ana Isabel Loureiro, and Patrício Soares da Silva. Computation of the binding affinities of catechol-O-methyltransferase inhibitors: Multisubstate relative free energy calculations. *Journal of Computational Chemistry*, 33(9):970–986, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Park:2019:GSA

[PBLS19] Taeyong Park, Minkyung Baek, Hasup Lee, and Chaok Seok. GalaxyTongDock: Symmetric and asymmetric ab initio protein-protein docking web server with improved energy parameters. *Journal of Computational Chemistry*, 40(27):2413–2417, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patra:2011:ANN

[PC11] Jagdish C. Patra and Boon H. Chua. Artificial neural network-based drug design for diabetes mellitus using flavonoids. *Journal of Computational Chemistry*, 32(4):555–567, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pelloni:2014:CCS

[PC14] Stefano Pelloni and Inmaculada García Cuesta. CCSD–CTOCD static dipole shielding polarizability for quantification of the chiral NMR effects in oxaziridine derivatives. *Journal of Computational Chemistry*, 35(25):1815–1823, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pritchard:2016:HVE

[PC16] Benjamin P. Pritchard and Edmond Chow. Horizontal vectorization of electron repulsion integrals. *Journal of Computational Chemistry*, 37(28):2537–2546, October 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pelloni:2011:RCM

[PCLL11] Stefano Pelloni, Raphaël Carion, Vincent Liégeois, and Paolo Lazzeretti. The ring current model of the pentaprismane molecule. *Journal of Computational Chemistry*, 32(8):1599–1611, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plumley:2011:CBF

[PD11] Joshua A. Plumley and J. J. Dannenberg. A comparison of the behavior of functional/basis set combinations for hydrogen-bonding in the water dimer with emphasis on basis set superposition error. *Journal of Computational Chemistry*, 32(8): 1519–1527, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plazinski:2012:DCI

[PD12] Wojciech Plazinski and Mateusz Drach. The dynamics of the calcium-induced chain–chain association in the polyuronate systems. *Journal of Computational Chemistry*, 33(20):1709–1715, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pinjari:2016:CSR

[PDG+16] Rahul V. Pinjari, Mickaël G. Delcey, Meiyuan Guo, Michael Odelius, and Marcus Lundberg. Cost and sensitivity of restricted active-space calculations of metal L-edge X-ray absorption spectra. *Journal of Computational Chemistry*, 37 (5):477–486, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Parac:2010:QMC

[PDMT10] Maja Parac, Markus Doerr, Christel M. Marian, and Walter Thiel. QM/MM calculation of solvent effects on absorption spectra of guanine. *Journal of Computational Chemistry*, 31 (1):90–106, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pansini:2018:MUE

[PdSC18] F. N. N. Pansini, F. A. L. de Souza, and C. T. Campos. Molecules under external electric field: On the changes in the electronic structure and validity limits of the theoretical predictions. *Journal of Computational Chemistry*, 39(20):1561–1567, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

PintoDaSilva:2011:TMC

[PE11] Luís Pinto Da Silva and Joaquim C. G. Esteves Da Silva. Theoretical modulation of the color of light emitted by firefly oxyluciferin. *Journal of Computational Chemistry*, 32(12): 2654–2663, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petrella:2011:VMS

[Pet11] Robert J. Petrella. A versatile method for systematic conformational searches: Application to CheY. *Journal of Computational Chemistry*, 32(11):2369–2385, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pedregal:2019:GAE

[PFAS+19] Jaime Rodríguez-Guerra Pedregal, Ignacio Funes-Ardoiz, Giuseppe Sciortino, José-Emilio Sánchez-Aparicio, Gregori Ujaque, Agustí Lledós, Jean-Didie Maréchal, and Feliu Maseras. GARLEEK: Adding an extra flavor to ONIOM. *Journal of Computational Chemistry*, 40(2):381–386, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pol-Fachin:2014:EVG

[PFVL14] Laercio Pol-Fachin, Hugo Verli, and Roberto D. Lins. Extension and validation of the GROMOS $53A6_{glyc}$ parameter set for glycoproteins. *Journal of Computational Chemistry*, 35

(29):2087–2095, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Popov:2014:SNU

[PG14] Petr Popov and Sergei Grudinin. Software news and updates: Rapid determination of RMSDs corresponding to macromolecular rigid body motions. *Journal of Computational Chemistry*, 35(12):950–956, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pavlova:2015:PMA

[PG15] Anna Pavlova and James C. Gumbart. Parametrization of macrolide antibiotics using the force field toolkit. *Journal of Computational Chemistry*, 36(27):2052–2063, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Parida:2018:NIP

[PG18] Rakesh Parida and Santanab Giri. Negative influence of p K_a on activation energy barrier: a case study for double proton transfer reaction in inorganic acid dimers. *Journal of Computational Chemistry*, 39(16):993–998, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2012:CSH

[PGC12] Sudip Pan, Santanab Giri, and Pratim K. Chattaraj. A computational study on the hydrogen adsorption capacity of various lithium-doped boron hydrides. *Journal of Computational Chemistry*, 33(4):425–434, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pacios:2012:CSL

[PGCT$^+$12] Luis F. Pacios, Cristina Gómez-Casado, Leticia Tordesillas, Arantxa Palacín, Rosa Sánchez-Monge, and Araceli Díaz-Perales. Computational study of ligand binding in lipid transfer proteins: Structures, interfaces, and free energies of protein-lipid complexes. *Journal of Computational Chemistry*, 33(22):1831–1844, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Paschoal:2016:PPN

[PGdO$^+$16] D. Paschoal, C. Fonseca Guerra, M. A. L. de Oliveira, T. C. Ramalho, and H. F. Dos Santos. Predicting Pt-195 NMR chemical shift using new relativistic all-electron basis set. *Journal of Computational Chemistry*, 37(26):2360–2373, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Park:2019:USC

[PGI19] Soohyung Park, Kerney J. Glover, and Wonpil Im. U-shaped caveolin-1 conformations are tightly regulated by hydrogen bonds with lipids. *Journal of Computational Chemistry*, 40 (16):1570–1577, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Popov:2019:CAR

[PGK+19] Petr Popov, Sergei Grudinin, Andrii Kurdiuk, Pavel Buslaev, and Stephane Redon. Controlled-advancement rigid-body optimization of nanosystems. *Journal of Computational Chemistry*, 40(27):2391–2399, October 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pantazes:2015:SNU

[PGL+15] Robert J. Pantazes, Matthew J. Grisewood, Tong Li, Nathanael P. Gifford, and Costas D. Maranas. Software news and updates: The Iterative Protein Redesign and Optimization (IPRO) suite of programs. *Journal of Computational Chemistry*, 36(4):251–263, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2015:CCS

[PGS+15] Sudip Pan, Ashutosh Gupta, Ranajit Saha, Gabriel Merino, and Pratim K. Chattaraj. A coupled-cluster study on the noble gas binding ability of metal cyanides versus metal halides (metal = Cu, Ag, Au). *Journal of Computational Chemistry*, 36(29):2168–2176, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pirojsirikul:2017:CQM

[PGW+17] Teerapong Pirojsirikul, Andreas W. Götz, John Weare, Ross C. Walker, Karol Kowalski, and Marat Valiev. Combined quantum-mechanical molecular mechanics calculations with NWChem and AMBER: Excited state properties of green fluorescent protein chromophore analogue in aqueous solution. *Journal of Computational Chemistry*, 38(18):1631–1639, July

5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Panteva:2015:CST

[PGY15] Maria T. Panteva, George M. Giambasu, and Darrin M. York. Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg^{2+} ion models commonly used in biomolecular simulations. *Journal of Computational Chemistry*, 36(13):970–982, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pesonen:2010:PCI

[PH10a] Janne Pesonen and Krister O. E. Henriksson. Polymer conformations in internal (polyspherical) coordinates. *Journal of Computational Chemistry*, 31(9):1873–1881, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Poolmee:2010:IES

[PH10b] Potjaman Poolmee and Supa Hannongbua. Investigation of excited-state properties of fluorene–thiophene oligomers by the SAC–CI theoretical approach. *Journal of Computational Chemistry*, 31(10):1945–1955, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Panosetti:2012:AMC

[PH12] Chiara Panosetti and Werner A. Hofer. Adsorption of metadiiodobenzene on Cu(110): a theoretical study. *Journal of Computational Chemistry*, 33(19):1623–1631, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Proppe:2015:CTM

[PH15] Jonny Proppe and Carmen Herrmann. Communication through molecular bridges: Different bridge orbital trends result in common property trends. *Journal of Computational Chemistry*, 36(4):201–209, February 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Passler:2017:CLM

[PH17] Peter P. Passler and Thomas S. Hofer. Conserving the linear momentum in stochastic dynamics: Dissipative particle dynamics as a general strategy to achieve local thermostatization in molecular dynamics simulations. *Journal of Computational Chemistry*, 38(5):265–275, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pang:2013:SEM

[PHC13] Xueqin Pang, Keli Han, and Qiang Cui. A simple but effective modeling strategy for structural properties of non-heme Fe(II) sites in proteins: Test of force field models and application to proteins in the AlkB family. *Journal of Computational Chemistry*, 34(19):1620–1635, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pape:2013:DDM

[PHDH13] Susanne Pape, Franziska Hoffgaard, Mirjam Dür, and Kay Hamacher. Distance dependency and minimum amino acid alphabets for decoy scoring potentials. *Journal of Computational Chemistry*, 34(1):10–20, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pool:2012:SNU

[PHH+12] René Pool, Jaap Heringa, Martin Hoefling, Roland Schulz, Jeremy C. Smith, and K. Anton Feenstra. Software news and updates: Enabling grand-canonical Monte Carlo: Extending the flexibility of GROMACS through the GromPy Python interface module. *Journal of Computational Chemistry*, 33 (12):1207–1214, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pedersen:2014:BSE

[PHK14] Morten N. Pedersen, Erik D. Hedegård, and Jacob Kongsted. Basis set error estimation for DFT calculations of electronic g-tensors for transition metal complexes. *Journal of Computational Chemistry*, 35(25):1809–1814, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pohl:2017:OSF

[PHT17] Vincent Pohl, Gunter Hermann, and Jean Christophe Tremblay. An open-source framework for analyzing N-electron dynamics. I. Multideterminantal wave functions. *Journal of Computational Chemistry*, 38(17):1515–1527, June 30, 2017.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pierens:2014:NSF

[Pie14] Gregory K. Pierens. ^{1}H and ^{13}C NMR scaling factors for the calculation of chemical shifts in commonly used solvents using density functional theory. *Journal of Computational Chemistry*, 35(18):1388–1394, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pilme:2017:ELF

[Pil17] Julien Pilmé. Electron localization function from density components. *Journal of Computational Chemistry*, 38(4):204–210, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Porta:2013:EEL

[PJ13] Josep M. Porta and Léonard Jaillet. Exploring the energy landscapes of flexible molecular loops using higher-dimensional continuation. *Journal of Computational Chemistry*, 34(3):234–244, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patel:2019:SNA

[PK19] Lara A. Patel and James T. Kindt. Simulations of NaCl aggregation from solution: Solvent determines topography of free energy landscape. *Journal of Computational Chemistry*, 40(1):135–147, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pissurlenkar:2011:EQQ

[PKIC11] Raghuvir R. S. Pissurlenkar, Vijay M. Khedkar, Radhakrishnan P. Iyer, and Evans C. Coutinho. Ensemble QSAR: a QSAR method based on conformational ensembles and metric descriptors. *Journal of Computational Chemistry*, 32(10): 2204–2218, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Papp:2017:TIN

[PKK17] Tamara Papp, László Kollár, and Tamás Kégl. Theoretical insights into the nature of Pt–Sn bond: Reevaluating the bonding/back-bonding properties of trichlorostannate with comparison to the cyano ligand. *Journal of Computational Chemistry*, 38(19):1712–1726, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pezeshki:2014:MDS

[PL14] Soroosh Pezeshki and Hai Lin. Molecular dynamics simulations of ion solvation by flexible-boundary QM/MM: On-the-fly partial charge transfer between QM and MM subsystems. *Journal of Computational Chemistry*, 35(24):1778–1788, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pelloni:2018:PCM

[PL18] Stefano Pelloni and Paolo Lazzeretti. Polygonal current models for polycyclic aromatic hydrocarbons and graphene sheets of various shapes. *Journal of Computational Chemistry*, 39 (1):21–34, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pei:2019:FVC

[PL19] Han-Wen Pei and Aatto Laaksonen. Feature vector clustering molecular pairs in computer simulations. *Journal of Computational Chemistry*, 40(29):2539–2549, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plazinski:2011:MBC

[Pla11] Wojciech Plazinski. Molecular basis of calcium binding by polyguluronate chains. Revising the egg-box model. *Journal of Computational Chemistry*, 32(14):2988–2995, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plewczynski:2011:CWT

[PŁAG11] Dariusz Plewczynski, Michał Łaźniewski, Rafał Augustyniak, and Krzysztof Ginalski. Can we trust docking results? Evaluation of seven commonly used programs on PDBbind database. *Journal of Computational Chemistry*, 32(4):742–755, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pagola:2018:IRE

[PLFS18] Gabriel I. Pagola, Martin A. B. Larsen, Marta Ferraro, and Stephan P. A. Sauer. The influence of relativistic effects on nuclear magnetic resonance spin-spin coupling constant polarizabilities of H_2 O_2, H_2 S_2, H_2 Se_2, and H_2 Te_2. *Journal of Computational Chemistry*, 39(31):2589–2600, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plazinski:2016:RGF

[PLH16] Wojciech Plazinski, Alice Lonardi, and Philippe H. Hünenberger. Revision of the GROMOS 56A6$_{CARBO}$ force field: Improving the description of ring-conformational equilibria in hexopyranose-based carbohydrates chains. *Journal of Computational Chemistry*, 37(3):354–365, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Presti:2016:MEF

[PLP+16] Davide Presti, Frédéric Labat, Alfonso Pedone, Michael J. Frisch, Hrant P. Hratchian, Ilaria Ciofini, Maria Cristina Menziani, and Carlo Adamo. Modeling emission features of salicylidene aniline molecular crystals: a QM/QM' approach. *Journal of Computational Chemistry*, 37(9):861–870, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plewczynski:2011:VCD

[PŁV+11] Dariusz Plewczynski, Michał Łażniewski, Marcin Von Grotthuss, Leszek Rychlewski, and Krzysztof Ginalski. VoteDock: Consensus docking method for prediction of protein–ligand interactions. *Journal of Computational Chemistry*, 32(4):568–581, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pang:2017:GAM

[PLZ17] Yujia Pang, Wenliang Li, and Jingping Zhang. Gas adsorption in Mg-porphyrin-based porous organic frameworks: a computational simulation by first-principles derived force field. *Journal of Computational Chemistry*, 38(24):2100–2107, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

PiEkos:2013:TDD

[PM13] Łukasz PiEkoś and Mariusz Paweł Mitoraj. Theoretical description of dihydrogen/hydride and trihydride molybdocene complexes: an insight from static and molecular dynamics simulations. *Journal of Computational Chemistry*, 34(4):294–304, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Politzer:2018:HHS

[PM18a] Peter Politzer and Jane S. Murray. σ-holes and π-holes: Similarities and differences. *Journal of Computational Chemistry*, 39(9):464–471, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Polkosnik:2018:SDR

[PM18b] Walter Polkosnik and Lou Massa. Single determinant N-representability and the kernel energy method applied to water clusters. *Journal of Computational Chemistry*, 39(17): 1038–1043, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pagliai:2017:EAS

[PMC+17] Marco Pagliai, Giordano Mancini, Ivan Carnimeo, Nicola De Mitri, and Vincenzo Barone. Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach. *Journal of Computational Chemistry*, 38(6):319–335, March 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2016:SSN

[PMG+16] Sudip Pan, Diego Moreno, Sreyan Ghosh, Pratim K. Chattaraj, and Gabriel Merino. Structure and stability of noble gas bound EX_3^+ compounds (E = C, Ge, Sn, Pb; X = H, F, Cl, Br). *Journal of Computational Chemistry*, 37(2):226–236, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Paschoal:2012:RBS

[PML+12] Diego Paschoal, Bruna L. Marcial, Juliana Fedoce Lopes, Wagner B. De Almeida, and Hélio F. Dos Santos. The role of the basis set and the level of quantum mechanical theory in the prediction of the structure and reactivity of cisplatin. *Journal of Computational Chemistry*, 33(29):2292–2302, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pomogaeva:2016:TCL

[PMT16] Anna V. Pomogaeva, Keiji Morokuma, and Alexey Y. Timoshkin. Trimeric cluster of lithium amidoborane — the smallest unit for the modeling of hydrogen release mechanism. *Journal of Computational Chemistry*, 37(14):1259–1264, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pipek:2013:EPR

[PN13] János Pipek and Szilvia Nagy. An economic prediction of refinement coefficients in wavelet-based adaptive methods for electron structure calculations. *Journal of Computational Chemistry*, 34(6):460–465, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petkovic:2018:WHM

[PNE18] Milena Petković, Dura Nakarada, and Mihajlo Etinski. When hydroquinone meets methoxy radical: Hydrogen abstraction reaction from the viewpoint of interacting quantum atoms. *Journal of Computational Chemistry*, 39(23):1868–1877, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Project:2010:FFD

[PNG10] Elad Project, Esther Nachliel, and Menachem Gutman. Force field-dependant structural divergence revealed during long time simulations of Calbindin d9k. *Journal of Computational Chemistry*, 31(9):1864–1872, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Perrin:2013:CSR

[PNI13] Bradley Scott Perrin Jr., Shuqiang Niu, and Toshiko Ichiye. Calculating standard reduction potentials of [4Fe–4S] proteins. *Journal of Computational Chemistry*, 34(7):576–582, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petraglia:2016:BSS

[PNW+16] Riccardo Petraglia, Adrien Nicolaï, Matthew D. Wodrich, Michele Ceriotti, and Clemence Corminboeuf. Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. *Journal of Computational Chemistry*, 37(1):83–92, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Peintinger:2013:CGB

[POB13] Michael F. Peintinger, Daniel Vilela Oliveira, and Thomas Bredow. Consistent Gaussian basis sets of triple-zeta valence with polarization quality for solid-state calculations. *Journal of Computational Chemistry*, 34(6):451–459, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pogliani:2010:MTP

[Pog10] Lionello Pogliani. Model of twelve properties of a set of organic solvents with graph-theoretical and/or experimental parameters. *Journal of Computational Chemistry*, 31(2):295–307, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Polestshuk:2013:AIA

[Pol13] Pavel M. Polestshuk. Accurate integration over atomic regions bounded by zero-flux surfaces. *Journal of Computational Chemistry*, 34(3):206–219, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pongsai:2010:CMM

[Pon10] Suchaya Pongsai. Combination of the Metropolis Monte Carlo and Lattice Statics method for geometry optimization of H-(Al)-ZSM-5. *Journal of Computational Chemistry*, 31(10): 1979–1985, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ponec:2011:BIS

[Pon11] Robert Ponec. Bond indices in solids: Extended analytical model. *Journal of Computational Chemistry*, 32(14):3114–3121, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Popelier:2018:FAI

[Pop18] Paul L. A. Popelier. A fully analytical integration of properties over the 3D volume of the β sphere in topological atoms. *Journal of Computational Chemistry*, 39(10):604–613, April 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Palfi:2010:SHL

[PP10] Villő K. Pálfi and András Perczel. Stability of the hydration layer of tropocollagen: a QM study. *Journal of Computational Chemistry*, 31(4):764–777, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Paul:2019:MDS

[PP19] Srijita Paul and Sandip Paul. Molecular dynamics simulation study on the inhibitory effects of choline-O-sulfate on hIAPP protofibrilation. *Journal of Computational Chemistry*, 40(22): 1957–1968, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pham:2014:DFT

[PPH+14] My-Phuong Pham, Buu Q. Pham, Lam K. Huynh, Ha Q. Pham, Maurice J. Marks, and Thanh N. Truong. Density functional theory study on mechanisms of epoxy-phenol curing reaction. *Journal of Computational Chemistry*, 35(22): 1630–1640, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plazinska:2014:FMB

[PPJ14] Anita Plazinska, Wojciech Plazinski, and Krzysztof Jozwiak. Fast, metadynamics-based method for prediction of the stereochemistry-dependent relative free energies of ligand–receptor interactions. *Journal of Computational Chemistry*, 35(11):876–882, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ponce:2015:SNU

[PPM15] Hiram Ponce, Pedro Ponce, and Arturo Molina. Software news and updates: The development of an artificial organic networks toolkit for LabVIEW. *Journal of Computational Chemistry*, 36(7):478–492, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prado-Prado:2010:UQN

[PPUBGD10] Francisco J. Prado-Prado, Florencio M. Ubeira, Fernanda Borges, and Humberto González-Díaz. Unified QSAR & network-based computational chemistry approach to antimicrobials. II. Multiple distance and triadic census analysis of antiparasitic drugs complex networks. *Journal of Computational Chemistry*, 31(1):164–173, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Papp:2017:FFI

[PRJ+17] Dóra Papp, Petra Rovó, Imre Jákli, Attila G. Császár, and András Perczel. Four faces of the interaction between ions and aromatic rings. *Journal of Computational Chemistry*, 38(20): 1762–1773, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Procacci:2016:REC

[Pro16] Piero Procacci. Reformulating the entropic contribution in molecular docking scoring functions. *Journal of Computational Chemistry*, 37(19):1819–1827, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Padhi:2015:PSH

[PRP15] Siladitya Padhi, Siddabattula Ramakrishna, and U. Deva Priyakumar. Prediction of the structures of helical membrane proteins based on a minimum unfavorable contacts approach. *Journal of Computational Chemistry*, 36(8):539–552, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Preat:2010:PTP

[PRRT+10] Julien Preat, Francisco Rodríguez-Ropero, Juan Torras, Oscar Bertran, David Zanuy, and Carlos Alemán. Parameterization of the torsional potential for calix[4]arene-substituted poly(thiophene)s. *Journal of Computational Chemistry*, 31 (8):1741–1751, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pfleger:2013:GLI

[PRSG13] Christopher Pfleger, Sebastian Radestock, Elena Schmidt, and Holger Gohlke. Global and local indices for characterizing biomolecular flexibility and rigidity. *Journal of Computa-*

tional Chemistry, 34(3):220–233, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pino-Rios:2017:PSE

[PRYI+17] Ricardo Pino-Rios, Osvaldo Yañez, Diego Inostroza, Lina Ruiz, Carlos Cardenas, Patricio Fuentealba, and William Tiznado. Proposal of a simple and effective local reactivity descriptor through a topological analysis of an orbital-weighted Fukui function. *Journal of Computational Chemistry*, 38(8): 481–488, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prakash:2010:FFD

[PS10] Priyanka Prakash and Ramasubbu Sankararamakrishnan. Force field dependence of phospholipid headgroup and acyl chain properties: Comparative molecular dynamics simulations of DMPC bilayers. *Journal of Computational Chemistry*, 31(2):266–277, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Polydorides:2013:MCS

[PS13] Savvas Polydorides and Thomas Simonson. Monte Carlo simulations of proteins at constant pH with generalized Born solvent, flexible sidechains, and an effective dielectric boundary. *Journal of Computational Chemistry*, 34(31):2742–2756, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Purushotham:2014:CCA

[PS14] Uppula Purushotham and G. Narahari Sastry. A comprehensive conformational analysis of tryptophan, its ionic and dimeric forms. *Journal of Computational Chemistry*, 35(8): 595–610, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Piccardo:2017:FPA

[PS17] Matteo Piccardo and Alessandro Soncini. A full-pivoting algorithm for the Cholesky decomposition of two-electron repulsion and spin-orbit coupling integrals. *Journal of Computational Chemistry*, 38(32):2775–2783, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Phillips:2011:MCO

[PSC11] Kathy L. Phillips, Stanley I. Sandler, and Pei C. Chiu. A method to calculate the one-electron reduction potentials for nitroaromatic compounds based on gas-phase quantum mechanics. *Journal of Computational Chemistry*, 32(2):226–239, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Planche:2010:DNA

[PSdPE+10] Alejandro Speck Planche, Marcus Tulius Scotti, Vicente de Paulo Emerenciano, América García López, Enrique Molina Pérez, and Eugenio Uriarte. Designing novel antitrypanosomal agents from a mixed graph-theoretical substructural approach. *Journal of Computational Chemistry*, 31(4):882–894, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pedregal:2017:SNU

[PSG+17] Jaime Rodríguez-Guerra Pedregal, Giuseppe Sciortino, Jordi Guasp, Martí Municoy, and Jean-Didier Maréchal. Software news and updates: GaudiMM: a modular multi-objective platform for molecular modeling. *Journal of Computational Chemistry*, 38(24):2118–2126, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pierdominici-Sottile:2015:NIM

[PSP15] Gustavo Pierdominici-Sottile and Juliana Palma. New insights into the meaning and usefulness of principal component analysis of concatenated trajectories. *Journal of Computational Chemistry*, 36(7):424–432, March 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Panshenskov:2014:SNU

[PSS14] Mikhail Panshenskov, Ilia A. Solov'yov, and Andrey V. Solov'yov. Software news and updates: Efficient 3D kinetic Monte Carlo method for modeling of molecular structure and dynamics. *Journal of Computational Chemistry*, 35(17):1317–1329, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plasser:2015:SAE

[PTB+15] Felix Plasser, Benjamin Thomitzni, Stefanie A. Bäppler, Jan Wenzel, Dirk R. Rehn, Michael Wormit, and Andreas Dreuw. Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. *Journal of Computational Chemistry*, 36(21):1609–1620, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pankratyev:2011:HRG

[PTK11] Evgeniy Yu. Pankratyev, Artur R. Tulyabaev, and Leonard M. Khalilov. How reliable are GIAO calculations of ^{1}H and ^{13}C NMR chemical shifts? A statistical analysis and empirical corrections at DFT (PBE/3z) level. *Journal of Computational Chemistry*, 32(9):1993–1997, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prandi:2016:CCM

[PVAM16] Ingrid G. Prandi, Lucas Viani, Oliviero Andreussi, and Benedetta Mennucci. Combining classical molecular dynamics and quantum mechanical methods for the description of electronic excitations: the case of carotenoids. *Journal of Computational Chemistry*, 37(11):981–991, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Puranen:2010:ACD

[PVJ10] J. Santeri Puranen, Mikko J. Vainio, and Mark S. Johnson. Accurate conformation-dependent molecular electrostatic potentials for high-throughput in silico drug discovery. *Journal of Computational Chemistry*, 31(8):1722–1732, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pacifici:2013:HLI

[PVL+13] Leonardo Pacifici, Marco Verdicchio, Noelia Faginas Lago, Andrea Lombardi, and Alessandro Costantini. A high-level ab initio study of the N_2 + N_2 reaction channel. *Journal of Computational Chemistry*, 34(31):2668–2676, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Poger:2010:NFF

[PVM10] David Poger, Wilfred F. Van Gunsteren, and Alan E. Mark. A new force field for simulating phosphatidylcholine bilayers. *Journal of Computational Chemistry*, 31(6):1117–1125, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Purushotham:2012:CIC

[PVS12] Uppula Purushotham, Dolly Vijay, and G. Narahari Sastry. A computational investigation and the conformational analysis of dimers, anions, cations, and zwitterions of L-phenylalanine. *Journal of Computational Chemistry*, 33(1):44–59, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Popov:2013:SNU

[PVZ13] Alexander V. Popov, Yury N. Vorobjev, and Dmitry O. Zharkov. Software news and updates: MDTRA: a molecular dynamics trajectory analyzer with a graphical user interface. *Journal of Computational Chemistry*, 34(4):319–325, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plessow:2012:SNU

[PW12] Philipp Plessow and Florian Weigend. Software news and updates: Seminumerical calculation of the Hartree–Fock exchange matrix: Application to two-component procedures and efficient evaluation of local hybrid density functionals. *Journal of Computational Chemistry*, 33(7):810–816, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pang:2010:SOS

[PXXW10] Xian-Yong Pang, Bin Xing, Li-Qin Xue, and Gui-Chang Wang. Selective oxidation of styrene on an oxygen-adsorbed Cu(111): a comparison with Au(111). *Journal of Computational Chemistry*, 31(8):1618–1624, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pyykko:2013:REB

[Pyy13] Pekka Pyykkö. The RTAM electronic bibliography, version 17.0, on relativistic theory of atoms and molecules. *Journal* *of Computational Chemistry*, 34(31):2667, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petukh:2015:SIS

[PZA15] Marharyta Petukh, Min Zhang, and Emil Alexov. Statistical investigation of surface bound ions and further development of BION server to include pH and salt dependence. *Journal of Computational Chemistry*, 36(32):2381–2393, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pinsky:2013:CSA

[PZBA13] Mark Pinsky, Amir Zait, Maayan Bonjack, and David Avnir. Continuous symmetry analyses: C_{nv} and D_n measures of molecules, complexes, and proteins. *Journal of Computational Chemistry*, 34(1):2–9, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Peng:2016:FES

[PZCL16] Xiangda Peng, Yuebin Zhang, Huiying Chu, and Guohui Li. Free energy simulations with the AMOEBA polarizable force field and metadynamics on GPU platform. *Journal of Computational Chemistry*, 37(6):614–622, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Porta:2015:HHB

[PZM15] Paolo Della Porta, Riccardo Zanasi, and Guglielmo Monaco. Hydrogen–hydrogen bonding: the current density perspective. *Journal of Computational Chemistry*, 36(10):707–716, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quapp:2010:CNE

[QB10] Wolfgang Quapp and Josep Maria Bofill. A comment to the nudged elastic band method. *Journal of Computational Chemistry*, 31(13):2526–2531, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quapp:2011:RCS

[QB11] Wolfgang Quapp and Josep Maria Bofill. Reply to the comment by Sheppard and Henkelman on the nudged elastic band method. *Journal of Computational Chemistry*, 32(8):1772–1773, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SH11a].

Quapp:2016:RRT

[QB16] Wolfgang Quapp and Josep Maria Bofill. Reaction rates in a theory of mechanochemical pathways. *Journal of Computational Chemistry*, 37(27):2467–2478, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quartarolo:2012:TIB

[QCR12] Angelo Domenico Quartarolo, Sandro Giuseppe Chiodo, and Nino Russo. A TDDFT investigation of bay substituted perylenediimides: Absorption and intersystem crossing. *Journal of Computational Chemistry*, 33(11):1091–1100, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qi:2019:CGN

[QLKI19] Yifei Qi, Jumin Lee, Jeffery B. Klauda, and Wonpil Im. CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. *Journal of Computational Chemistry*, 40(7):893–899, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qi:2011:UHC

[QLQ11] Zhao-Hui Qi, Ling Li, and Xiao-Qin Qi. Using Huffman coding method to visualize and analyze DNA sequences. *Journal of Computational Chemistry*, 32(15):3233–3240, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qi:2010:DSA

[QLYL10] Na Qi, Rong-Zhen Liao, Jian-Guo Yu, and Ruo-Zhuang Liu. DFT study of the asymmetric nitroaldol (Henry) reaction catalyzed by a dinuclear Zn complex. *Journal of Computational Chemistry*, 31(7):1376–1384, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qian:2018:MIB

[QQY+18] Min Qian, Bowen Qin, Haiyan Yuan, Wenliang Li, and Jingping Zhang. Mechanistic insights into N-bromosuccinimidepromoted synthesis of imidazo[1,2-a]pyridine in water: Reactivity mediated by substrates and solvent. *Journal of Computational Chemistry*, 39(27):2324–2332, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quanz:2019:TEU

[QS19] Henrik Quanz and Peter R. Schreiner. TUNNEX: an easy-to-use Wentzel–Kramers–Brillouin (WKB) implementation to compute tunneling half-lives. *Journal of Computational Chemistry*, 40(2):543–547, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qu:2010:RPP

[QSW+10] Yena Qu, Kehe Su, Xin Wang, Yan Liu, Qingfeng Zeng, Laifei Cheng, and Litong Zhang. Reaction pathways of propene pyrolysis. *Journal of Computational Chemistry*, 31(7):1421–1442, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qian:2010:CCP

[QZ10a] Jianguo Qian and Fuji Zhang. Counting the cyclocized polyphenacenes. *Journal of Computational Chemistry*, 31 (14):2577–2584, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qu:2010:DAT

[QZ10b] Zheng-Wang Qu and Hui Zhu. Do anionic titanium dioxide nano-clusters reach bulk band gap? A density functional theory study. *Journal of Computational Chemistry*, 31(10): 2038–2045, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quapp:2010:TST

[QZ10c] Wolfgang Quapp and Alraune Zech. Transition state theory with Tsallis statistics. *Journal of Computational Chemistry*, 31(3):573–585, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qu:2011:VSS

[QZM11] Zheng-Wang Qu, Hui Zhu, and Volkhard May. Vibrational spectral signatures of peptide secondary structures: *N*-methylation and side chain hydrogen bond in cyclosporin A.

Journal of Computational Chemistry, 32(8):1500–1518, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rabilloud:2012:SSC

[Rab12] F. Rabilloud. Structure and stability of coinage metal fluoride and chloride clusters (M_nF_n and M_nCl_n, M = Cu, Ag, or Au; $n = 1$–6). *Journal of Computational Chemistry*, 33(26):2083–2091, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramirez-Anguita:2011:VTS

[RAGLL11] Juan M. Ramírez-Anguita, Àngels González-Lafont, and José M. Lluch. Variational transition-state theory study of the rate constant of the DMS·OH scavenging reaction by O_2. *Journal of Computational Chemistry*, 32(10):2104–2118, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2012:VES

[Ran12] M. Randić. Very Efficient Search for Protein Alignment — VESPA. *Journal of Computational Chemistry*, 33(6):702–707, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2013:VES

[Ran13] Milan Randić. Very efficient search for nucleotide alignments. *Journal of Computational Chemistry*, 34(2):77–82, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2019:BRR

[Ran19] Milan Randić. Benzenoid rings resonance energies and local aromaticity of benzenoid hydrocarbons. *Journal of Computational Chemistry*, 40(5):753–762, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rao:2011:PIS

[Rao11] Francesco Rao. Protein inherent structures by different minimization strategies. *Journal of Computational Chemistry*, 32(6):1113–1116, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rathore:2011:MMS

[RAR+11] R. S. Rathore, P. Aparoy, P. Reddanna, A. K. Kondapi, and M. Rami Reddy. Minimum MD simulation length required to achieve reliable results in free energy perturbation calculations: Case study of relative binding free energies of fructose-1,6-bisphosphatase inhibitors. *Journal of Computational Chemistry*, 32(10):2097–2103, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raskovalov:2017:SNU

[Ras17] Anton Raskovalov. Software news and updates: a new extension of classical molecular dynamics: an electron transfer algorithm. *Journal of Computational Chemistry*, 38(12):926–932, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rayne:2013:LEC

[Ray13] Sierra Rayne. Letters to the editor: Comment on "QSAR model reproducibility and applicability: a case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzo-)triazoles". *Journal of Computational Chemistry*, 34(20):1794–1795, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [RKG11, GKR13].

Ricci:2012:DFT

[RB12] Antonio Ricci and Andrea Brancale. Density functional theory calculation of cyclic carboxylic phosphorus mixed anhydrides as possible intermediates in biochemical reactions: Implications for the Pro-Tide approach. *Journal of Computational Chemistry*, 33(10):1029–1037, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rai:2013:FAG

[RB13a] Brajesh K. Rai and Gregory A. Bakken. Fast and accurate generation of ab initio quality atomic charges using nonparametric statistical regression. *Journal of Computational Chemistry*, 34(19):1661–1671, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rice:2013:EED

[RB13b] Betsy M. Rice and Edward F. C. Byrd. Evaluation of electrostatic descriptors for predicting crystalline density. *Journal of Computational Chemistry*, 34(25):2146–2151, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Robinson:2011:WOP

[RBOH11] David Robinson, Nicholas A. Besley, Paul O'Shea, and Jonathan D. Hirst. Water order profiles on phospholipid/cholesterol membrane bilayer surfaces. *Journal of Computational Chemistry*, 32(12):2613–2618, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roe:2018:PCE

[RC18] Daniel R. Roe and Thomas E. Cheatham III. Parallelization of CPPTRAJ enables large scale analysis of molecular dynamics trajectory data. *Journal of Computational Chemistry*, 39(25):2110–2117, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ren:2013:UEE

[RCM+13a] Yanliang Ren, Bo Chi, Osama Melhem, Ke Wei, Lingling Feng, Yongjian Li, Xinya Han, Ding Li, Ying Zhang, Jian Wan, Xin Xu, and Minghui Yang. Understanding the electronic energy transfer pathways in the trimeric and hexameric aggregation state of cyanobacteria phycocyanin within the framework of förster theory. *Journal of Computational Chemistry*, 34(12):1005–1012, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roy:2013:SNU

[RCM+13b] Kunal Roy, Pratim Chakraborty, Indrani Mitra, Probir Kumar Ojha, Supratik Kar, and Rudra Narayan Das. Software news and updates: Some case studies on application of "r_m^2" metrics for judging quality of quantitative structure–activity relationship predictions: Emphasis on scaling of response data. *Journal of Computational Chemistry*, 34(12):1071–1082, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rao:2016:DNC

[RCR+16] Li Rao, Bo Chi, Yanliang Ren, Yongjian Li, Xin Xu, and Jian Wan. DOX: a new computational protocol for accurate prediction of the protein–ligand binding structures. *Journal of Computational Chemistry*, 37(3):336–344, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rajendiran:2018:PBP

[RD18] Nivedita Rajendiran and Jacob D. Durrant. Pyrite: a `blender` plugin for visualizing molecular dynamics simulations using industry-standard rendering techniques. *Journal of Computational Chemistry*, 39(12):748–755, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ribeiro:2012:SNU

[RdA12] André A. S. T. Ribeiro and Ricardo B. de Alencastro. Software news and updates: Mixed Monte Carlo/molecular dynamics simulations in explicit solvent. *Journal of Computational Chemistry*, 33(8):901–905, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rastelli:2010:FAP

[RDDS10] Giulio Rastelli, Alberto Del Rio, Gianluca Degliesposti, and Miriam Sgobba. Fast and accurate predictions of binding free energies using MM-PBSA and MM-GBSA. *Journal of Computational Chemistry*, 31(4):797–810, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ravelli:2011:PUS

[RDF+11] Davide Ravelli, Daniele Dondi, Maurizio Fagnoni, Angelo Albini, and Alessandro Bagno. Predicting the UV spectrum of polyoxometalates by TD-DFT. *Journal of Computational Chemistry*, 32(14):2983–2987, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roth:2016:HRE

[RDRC16] Christine-Andrea Roth, Tom Dreyfus, Charles H. Robert, and Frédéric Cazals. Hybridizing rapidly exploring random trees and basin hopping yields an improved exploration of energy landscapes. *Journal of Computational Chemistry*, 37(8):739–752, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raupach:2014:QIB

[RDT14] Marc Raupach, Stefanie Dehnen, and Ralf Tonner. Quantitative investigation of bonding characteristics in ternary Zintl anions: Charge and energy analysis of $[Sn_2\ E^{15}_2\ (ZnPh)]^-$ (E^{15} = Sb, Bi) and $[Sn_2\ Sb_5\ (ZnPh)_2]^{3-}$. *Journal of Computational Chemistry*, 35(14):1045–1057, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rybkin:2013:ICB

[REH13] Vladimir V. Rybkin, Ulf Ekström, and Trygve Helgaker. Internal-to-cartesian back transformation of molecular geometry steps using high-order geometric derivatives. *Journal of Computational Chemistry*, 34(21):1842–1849, August 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rossi:2014:CIS

[REL+14] Elda Rossi, Stefano Evangelisti, Antonio Laganà, Antonio Monari, Sergio Rampino, Marco Verdicchio, Kim K. Baldridge, Gian Luigi Bendazzoli, Stefano Borini, Renzo Cimiraglia, Celestino Angeli, Peter Kallay, Hans P. Lüthi, Kenneth Ruud, José Sanchez-Marin, Anthony Scemama, Peter G. Szalay, and Attila Tajti. Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, 35(8):611–621, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rombouts:2017:QAL

[REL17] Jeroen A. Rombouts, Andreas W. Ehlers, and Koop Lammertsma. A quantitative analysis of light-driven charge transfer processes using Voronoi partitioning of time dependent DFT-derived electron densities. *Journal of Computational Chemistry*, 38(20):1811–1818, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rubez:2017:GAI

[REV+17] Gaëtan Rubez, Jean-Matthieu Etancelin, Xavier Vigouroux, Michael Krajecki, Jean-Charles Boisson, and Eric Hénon.

GPU accelerated implementation of NCI calculations using promolecular density. *Journal of Computational Chemistry*, 38(14):1071–1083, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezac:2016:SNU

[Řez16] Jan Řezáč. Software news and updates: Cuby: an integrative framework for computational chemistry. *Journal of Computational Chemistry*, 37(13):1230–1237, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezac:2019:DHB

[Rez19] Jan Rezác. Description of halogen bonding in semiempirical quantum-mechanical and self-consistent charge density-functional tight-binding methods. *Journal of Computational Chemistry*, 40(17):1633–1642, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezabal:2015:EBE

[RF15] Elixabete Rezabal and Gilles Frison. Estimating π binding energy of *N*-heterocyclic carbenes: the role of polarization. *Journal of Computational Chemistry*, 36(8):564–572, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ruscio:2010:HHS

[RFHG10] Jory Z. Ruscio, Nicolas L. Fawzi, and Teresa Head-Gordon. How hot? Systematic convergence of the replica exchange method using multiple reservoirs. *Journal of Computational Chemistry*, 31(3):620–627, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Renison:2015:QSL

[RFN15] C. Alicia Renison, Kyle D. Fernandes, and Kevin J. Naidoo. Quantum supercharger library: Hyper-parallel integral derivatives algorithms for ab initio QM/ MM dynamics. *Journal of Computational Chemistry*, 36(18):1410–1419, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Robertson:2019:NSN

[RGVC$^+$19] Christopher Robertson, Jesús González-Vázquez, Ines Corral, Sergio Díaz-Tendero, and Cristina Díaz. Nonadiabatic scattering of NO off Au_3 clusters: a simple and robust diabatic state manifold generation method for multiconfigurational wavefunctions. *Journal of Computational Chemistry*, 40 (6):794–810, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raymond:2011:FAM

[RHJ11] John W. Raymond, Daniel D. Holsworth, and Mehran Jalaie. The flexible alignment of molecular structures using simulated annealing with weighted Lagrangian multipliers. *Journal of Computational Chemistry*, 32(2):210–217, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rafati:2010:CMC

[RHNN10] Amir Abbas Rafati, Sayed Majid Hashemianzadeh, Zabiollah Bolboli Nojini, and Negin Naghshineh. Canonical Monte Carlo simulation of adsorption of O_2 and N_2 mixture on single walled carbon nanotube at different temperatures and pressures. *Journal of Computational Chemistry*, 31(7):1443–1449, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rohrmuller:2013:BOP

[RHPWS13] M. Rohrmüller, S. Herres-Pawlis, M. Witte, and W. G. Schmidt. Bis-μ-oxo and μ-η^2:η^2-peroxo dicopper complexes studied within (time-dependent) density-functional and many-body perturbation theory. *Journal of Computational Chemistry*, 34(12):1035–1045, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Racine:2016:RWF

[RHRCH16] Julien Racine, Denis Hagebaum-Reignier, Yannick Carissan, and Stéphane Humbel. Recasting wave functions into valence bond structures: a simple projection method to describe excited states. *Journal of Computational Chemistry*, 37(8):771–779, March 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rohrmuller:2015:CTT

[RHT+15] Martin Rohrmüller, Alexander Hoffmann, Christian Thierfelder, Sonja Herres-Pawlis, and Wolf Gero Schmidt. The Cu_2 O_2 torture track for a real-life system: $[Cu_2\ (btmgp)_2O_2]^{2+}$

oxo and peroxo species in density functional calculations. *Journal of Computational Chemistry*, 36(22):1672–1685, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rui:2010:POP

[RI10] Huan Rui and Wonpil Im. Protegrin-1 orientation and physicochemical properties in membrane bilayers studied by potential of mean force calculations. *Journal of Computational Chemistry*, 31(16):2859–2867, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rick:2016:PCT

[Ric16] Steven W. Rick. A polarizable, charge transfer model of water using the Drude oscillator. *Journal of Computational Chemistry*, 37(22):2060–2066, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Re:2011:GAY

[RIJ+11] Suyong Re, Takashi Imai, Jaewoon Jung, Seiichiro Ten-No, and Yuji Sugita. Geometrically associative yet electronically dissociative character in the transition state of enzymatic reversible phosphorylation. *Journal of Computational Chemistry*, 32(2):260–270, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raeker:2018:SOS

[RJBH18] Tim Raeker, Björn Jansen, Dominik Behrens, and Bernd Hartke. Simulations of optically switchable molecular machines for particle transport. *Journal of Computational Chemistry*, 39(20):1433–1443, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reckien:2012:IED

[RJPB12] Werner Reckien, Florian Janetzko, Michael F. Peintinger, and Thomas Bredow. Implementation of empirical dispersion corrections to density functional theory for periodic systems. *Journal of Computational Chemistry*, 33(25):2023–2031, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ringholm:2014:GRO

[RJR14] Magnus Ringholm, Dan Jonsson, and Kenneth Ruud. A general, recursive, and open-ended response code. *Journal of Computational Chemistry*, 35(8):622–633, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rubesova:2017:EML

[RJS17] Martina Rubešová, Veronika Jurásková, and Petr Slavíček. Efficient modeling of liquid phase photoemission spectra and reorganization energies: Difficult case of multiply charged anions. *Journal of Computational Chemistry*, 38(7):427–437, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Riojas:2012:PAD

[RJWW12] Amanda G. Riojas, Joshua R. John, T. Gavin Williams, and Angela K. Wilson. Proton affinities of deoxyribonucleosides via the ONIOM-ccCA methodology. *Journal of Computational Chemistry*, 33(32):2590–2601, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rusakov:2015:FCR

[RK15] Yury Yu. Rusakov and Leonid B. Krivdin. Four-component relativistic DFT calculations of ^{77}Se NMR chemical shifts: a gateway to a reliable computational scheme for the medium-sized organoselenium molecules. *Journal of Computational Chemistry*, 36(23):1756–1762, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rossini:2016:EPS

[RK16a] Emanuele Rossini and Ernst-Walter Knapp. Erratum: Proton solvation in protic and aprotic solvents [J. Comput. Chem. 2015, 37, 1082–1091]. *Journal of Computational Chemistry*, 37(23):2163–2164, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [RK16b].

Rossini:2016:PSP

[RK16b] Emanuele Rossini and Ernst-Walter Knapp. Proton solvation in protic and aprotic solvents. *Journal of Computational Chemistry*, 37(12):1082–1091, May 5, 2016. CODEN

JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [RK16a].

Romero:2014:PDU

[RKB+14] Ariadna Blanca Romero, Piotr M. Kowalski, George Beridze, Hartmut Schlenz, and Dirk Bosbach. Performance of DFT+U method for prediction of structural and thermodynamic parameters of monazite-type ceramics. *Journal of Computational Chemistry*, 35(18):1339–1346, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roston:2014:SRM

[RKDM14] Daniel Roston, Amnon Kohen, Dvir Doron, and Dan T. Major. Simulations of remote mutants of dihydrofolate reductase reveal the nature of a network of residues coupled to hydride transfer. *Journal of Computational Chemistry*, 35(19):1411–1417, July 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roy:2011:QMR

[RKG11] Partha Pratim Roy, Simona Kovarich, and Paola Gramatica. QSAR model reproducibility and applicability: a case study of rate constants of hydroxyl radical reaction models applied to polybrominated diphenyl ethers and (benzo-)triazoles. *Journal of Computational Chemistry*, 32(11):2386–2396, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [Ray13] and reply [GKR13].

Rahalkar:2010:MTA

[RKGN10] Anuja P. Rahalkar, Michio Katouda, Shridhar R. Gadre, and Shigeru Nagase. Molecular tailoring approach in conjunction with MP2 and Ri-MP2 codes: a comparison with fragment molecular orbital method. *Journal of Computational Chemistry*, 31(13):2405–2418, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reis:2011:EVL

[RLA+11] H. Reis, O. Loboda, A. Avramopoulos, M. G. Papadopoulos, B. Kirtman, J. M. Luis, and R. Zaleśny. Electronic and vibrational linear and nonlinear polarizabilities of Li@C_{60} and [Li@C_{60}]$^+$. *Journal of Computational Chemistry*, 32(5):908–914, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Romanova:2018:EEN

[RLA18] Anna Romanova, Konstantin Lyssenko, and Ivan Ananyev. Estimations of energy of noncovalent bonding from integrals over interatomic zero-flux surfaces: Correlation trends and beyond. *Journal of Computational Chemistry*, 39(21):1607–1616, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roscioni:2012:DTC

[RLD12] Otello M. Roscioni, Edmond P. F. Lee, and John M. Dyke. Development and testing of a compact basis set for use in effective core potential calculations on rhodium complexes. *Journal of Computational Chemistry*, 33(26):2049–2057, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raman:2017:ERF

[RLDJ17] E. Prabhu Raman, Sirish Kaushik Lakkaraju, Rajiah Aldrin Denny, and Alexander D. MacKerell Jr. Estimation of relative free energies of binding using pre-computed ensembles based on the single-step free energy perturbation and the site-identification by ligand competitive saturation approaches. *Journal of Computational Chemistry*, 38(15):1238–1251, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rajamani:2011:OSM

[RLG11] Ramkumar Rajamani, Yen-Lin Lin, and Jiali Gao. The opsin shift and mechanism of spectral tuning in rhodopsin. *Journal of Computational Chemistry*, 32(5):854–865, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Romo:2014:LOO

[RLG14] Tod D. Romo, Nicholas Leioatts, and Alan Grossfield. Lightweight object oriented structure analysis: Tools for building tools to analyze molecular dynamics simulations. *Journal of Computational Chemistry*, 35(32):2305–2318, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rao:2010:ISM

[RLL+10] Hanbing Rao, Zerong Li, Xiangyuan Li, Xiaohua Ma, Choongyong Ung, Hu Li, Xianghui Liu, and Yuzong Chen. Identification of small molecule aggregators from large compound libraries by support vector machines. *Journal of Computational Chemistry*, 31(4):752–763, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rampino:2012:SNU

[RLLHL12] Sergio Rampino, Noelia Faginas Lago, Antonio Laganà, and Fermin Huarte-Larrañaga. Software news and updates: An extension of the grid empowered molecular simulator to quantum reactive scattering. *Journal of Computational Chemistry*, 33(6):708–714, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ricca:2018:BCG

[RLZ+18] Chiara Ricca, Frédéric Labat, Claudia Zavala, Nino Russo, Carlo Adamo, Gabriel Merino, and Emilia Sicilia. B,n-codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. *Journal of Computational Chemistry*, 39(11):637–647, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ruiz:2011:SEA

[RMGB11] Juan M. Ruiz, R. Joshua Mulder, Célia Fonseca Guerra, and F. Matthias Bickelhaupt. Steric effects on alkyl cation affinities of maingroup-element hydrides. *Journal of Computational Chemistry*, 32(4):681–688, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ren:2015:CIE

[RML+15] Yanliang Ren, Osama Melhem, Yongjian Li, Bo Chi, Xinya Han, Hao Zhu, Lingling Feng, Jian Wan, and Xin Xu. Clarifying and illustrating the electronic energy transfer pathways in trimeric and hexameric aggregation state of cyanobacteria allophycocyanin within the framework of Förster theory. *Journal of Computational Chemistry*, 36(3):137–145, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rehman:2016:SS

[RMM16] Habib U. Rehman, Nida A. McKee, and Michael L. McKee. Saturn systems. *Journal of Computational Chemistry*, 37(2): 194–209, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramirez-Manzanares:2015:HAM

[RMPAM15] Alonso Ramirez-Manzanares, Joaquin Peña, Jon M. Azpiroz, and Gabriel Merino. A hierarchical algorithm for molecular similarity (H-FORMS). *Journal of Computational Chemistry*, 36(19):1456–1466, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Romero-Molina:2019:PDS

[RMRBH+19] Sandra Romero-Molina, Yasser B. Ruiz-Blanco, Mirja Harms, Jan Münch, and Elsa Sanchez-Garcia. PPI-Detect: a support vector machine model for sequence-based prediction of protein-protein interactions. *Journal of Computational Chemistry*, 40(11):1233–1242, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rogers:2017:PDM

[RN17] Ian L. Rogers and Kevin J. Naidoo. Producing DFT/MM enzyme reaction trajectories from SCC-DFTB/MM driving forces to probe the underlying electronics of a glycosyltransferase reaction. *Journal of Computational Chemistry*, 38(20): 1789–1798, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2013:CVMa

[RNP13] Milan Randić, Marjana Novič, and Dejan Plavšić. Common vertex matrix: a novel characterization of molecular graphs by counting. *Journal of Computational Chemistry*, 34(16):1409–1419, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rosen:2019:IPM

[RNS19] Andrew S. Rosen, Justin M. Notestein, and Randall Q. Snurr. Identifying promising metal-organic frameworks for heterogeneous catalysis via high-throughput periodic density functional theory. *Journal of Computational Chemistry*, 40(12):

1305–1318, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramsey:2016:SNU

[RNSF+16] Steven Ramsey, Crystal Nguyen, Romelia Salomon-Ferrer, Ross C. Walker, Michael K. Gilson, and Tom Kurtzman. Software news and updates: Solvation thermodynamic mapping of molecular surfaces in AmberTools: GIST. *Journal of Computational Chemistry*, 37(21):2029–2037, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2013:CVMb

[RNVP13] Milan Randić, Marjana Novič, Marjan Vračko, and Dejan Plavšić. On the centrality of vertices of molecular graphs. *Journal of Computational Chemistry*, 34(29):2514–2523, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reif:2014:MDS

[RO14a] Maria M. Reif and Chris Oostenbrink. Molecular dynamics simulation of configurational ensembles compatible with experimental FRET efficiency data through a restraint on instantaneous FRET efficiencies. *Journal of Computational Chemistry*, 35(32):2319–2332, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reif:2014:NCC

[RO14b] Maria M. Reif and Chris Oostenbrink. Net charge changes in the calculation of relative ligand-binding free energies via classical atomistic molecular dynamics simulation. *Journal of Computational Chemistry*, 35(3):227–243, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Robinson:2013:SMB

[Rob13] David Robinson. Splitting multiple bonds: a comparison of methodologies on the accuracy of bond dissociation energies. *Journal of Computational Chemistry*, 34(30):2625–2634, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rodriguez:2013:EMC

[Rod13] Juan I. Rodríguez. An efficient method for computing the QTAIM topology of a scalar field: the electron density case. *Journal of Computational Chemistry*, 34(8):681–686, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2015:PAE

[RP15] Milan Randić and Tomaz Pisanski. Protein alignment: Exact versus approximate. An illustration. *Journal of Computational Chemistry*, 36(14):1069–1074, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2010:NGD

[RPNP10] Milan Randić, Tomaž Pisanski, Marjana Novič, and Dejan Plavšić. Novel graph distance matrix. *Journal of Computational Chemistry*, 31(9):1832–1841, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rubensson:2011:BAM

[RR11] Emanuel H. Rubensson and Elias Rudberg. Bringing about matrix sparsity in linear-scaling electronic structure calculations. *Journal of Computational Chemistry*, 32(7):1411–1423, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rokob:2012:CCM

[RR12] Tibor András Rokob and Lubomír Rulíšek. Curvature correction for microiterative optimizations with QM/MM electronic embedding. *Journal of Computational Chemistry*, 33(12):1197–1206, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Riahi:2014:SNU

[RR14] Saleh Riahi and Christopher N. Rowley. Software news and updates: The CHARMM–TURBOMOLE interface for efficient and accurate QM/MM molecular dynamics, free energies, and excited state properties. *Journal of Computational Chemistry*, 35(28):2076–2086, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rousse:2019:ISO

[RR19] François Rousse and Stéphane Redon. Incremental solver for orbital-free density functional theory. *Journal of Computational Chemistry*, 40(23):2013–2027, September 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ricca:2015:CDI

[RRC+15] Chiara Ricca, Armelle Ringuedé, Michel Cassir, Carlo Adamo, and Frederic Labat. A comprehensive DFT investigation of bulk and low-index surfaces of ZrO_2 polymorphs. *Journal of Computational Chemistry*, 36(1):9–21, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rodriguez-Ropero:2011:EMZ

[RRF11] Francisco Rodríguez-Ropero and Marco Fioroni. Effect of Na^+, Mg^{2+}, and Zn^{2+} chlorides on the structural and thermodynamic properties of water/n-heptane interfaces. *Journal of Computational Chemistry*, 32(9):1876–1886, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rodriguez:2018:TCA

[RRFV+18] Aurelio Rodríguez, Roberto Rodríguez-Fernández, Saulo A. Vázquez, George L. Barnes, James J. P. Stewart, and Emilio Martínez-Núñez. `tsscds2018`: a code for automated discovery of chemical reaction mechanisms and solving the kinetics. *Journal of Computational Chemistry*, 39(23):1922–1930, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezac:2012:EPP

[ŘRH12] Jan Řezáč, Kevin E. Riley, and Pavel Hobza. Evaluation of the performance of post-Hartree–Fock methods in terms of intermolecular distance in noncovalent complexes. *Journal of Computational Chemistry*, 33(6):691–694, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezapour:2014:MSU

[RRK14] Mohammad Reza Rezapour, Arunkumar Chitteth Rajan, and Kwang S. Kim. Molecular sensing using armchair graphene nanoribbon. *Journal of Computational Chemistry*, 35(26): 1916–1920, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rusakova:2016:FEC

[RRK16] Irina L. Rusakova, Yury Yu. Rusakov, and Leonid B. Krivdin. First example of the correlated calculation of the one-bond tellurium–carbon spin–spin coupling constants: Relativistic effects, vibrational corrections, and solvent effects. *Journal of Computational Chemistry*, 37(15):1367–1372, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rao:2012:TKL

[RS12] Francesco Rao and Martin Spichty. Thermodynamics and kinetics of large-time-step molecular dynamics. *Journal of Computational Chemistry*, 33(5):475–483, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Remya:2013:WDF

[RS13] Karunakaran Remya and Cherumuttathu H. Suresh. Which density functional is close to CCSD accuracy to describe geometry and interaction energy of small non-covalent dimers? A benchmark study using `gaussian09`. *Journal of Computational Chemistry*, 34(15):1341–1353, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Remya:2014:CCG

[RS14] Karunakaran Remya and Cherumuttathu H. Suresh. Cooperativity and cluster growth patterns in acetonitrile: a DFT study. *Journal of Computational Chemistry*, 35(12):910–922, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rakhi:2017:DSD

[RS17a] Ramachandran Rakhi and Cherumuttathu H. Suresh. A DFT study on 1,4-dihydro-1,4-azaborinine annulated linear polyacenes: Absorption spectra, singlet-triplet energy gap, aromaticity, and HOMO–LUMO energy modulation. *Journal of Computational Chemistry*, 38(26):2232–2240, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Remya:2017:TEB

[RS17b] Premaja R. Remya and Cherumuttathu H. Suresh. Theoretical evidence for bond stretch isomerism in Grubbs olefin metathesis. *Journal of Computational Chemistry*, 38(19): 1704–1711, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rybkin:2013:IDE

[RSB+13] Vladimir V. Rybkin, Anton O. Simakov, Vebjørn Bakken, Simen Reine, Thomas Kjærgaard, Trygve Helgaker, and Einar Uggerud. Insights into the dynamics of evaporation and proton migration in protonated water clusters from large-scale Born–Oppenheimer direct dynamics. *Journal of Computational Chemistry*, 34(7):533–544, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rzepiela:2010:RAD

[RSG+10] Andrzej J. Rzepiela, Lars V. Schäfer, Nicolae Goga, H. Jelger Risselada, Alex H. De Vries, and Siewert J. Marrink. Reconstruction of atomistic details from coarse-grained structures. *Journal of Computational Chemistry*, 31(6):1333–1343, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Risthaus:2014:ING

[RSG14] Tobias Risthaus, Marc Steinmetz, and Stefan Grimme. Implementation of nuclear gradients of range-separated hybrid density functionals and benchmarking on rotational constants for organic molecules. *Journal of Computational Chemistry*, 35(20):1509–1516, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ryzhikov:2015:SSR

[RSK+15] Maxim R. Ryzhikov, Vladimir A. Slepkov, Svetlana G. Kozlova, Svyatoslav P. Gabuda, and Vladimir E. Fedorov. Solid-state reaction as a mechanism of 1T $\leftrightarrow$ 2H transformation in MoS_2 monolayers. *Journal of Computational Chemistry*, 36

(28):2131–2134, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ryzhikov:2014:ECB

[RSKG14] Maxim R. Ryzhikov, Vladimir A. Slepkov, Svetlana G. Kozlova, and Svyatoslav P. Gabuda. Evolution of chemical bonding and electron density rearrangements during D_{3h} D_{3d} reaction in monolayered TiS_2: a QTAIM and ELF study. *Journal of Computational Chemistry*, 35(22):1641–1645, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ru:2016:GAE

[RSL16] Xiao Ru, Ce Song, and Zijing Lin. A genetic algorithm encoded with the structural information of amino acids and dipeptides for efficient conformational searches of oligopeptides. *Journal of Computational Chemistry*, 37(13):1214–1222, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roca-Sanjuan:2012:LEC

[RSLML12] Daniel Roca-Sanjuán, Marcus Lundberg, David A. Mazziotti, and Roland Lindh. Letters to the editor: Comment on "Density functional theory study of 1,2-dioxetanone decomposition in condensed phase". *Journal of Computational Chemistry*, 33(26):2124–2126, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [dSdS12a, dSdS12b].

Roberts:2013:LMH

[RSLS13] Elijah Roberts, John E. Stone, and Zaida Luthey-Schulten. Lattice microbes: High-performance stochastic simulation method for the reaction-diffusion master equation. *Journal of Computational Chemistry*, 34(3):245–255, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roberts:2012:SNU

[RSR+12] Benjamin P. Roberts, Gustavo M. Seabra, Adrian E. Roitberg, Kenneth M. Merz, Erik Deumens, Juan Torras, and Samuel B. Trickey. Software news and updates: Commentary: Comment on "A minimal implementation of the AMBER–GAUSSIAN interface for Ab Initio QM/MM-MD simulation".

Journal of Computational Chemistry, 33(19):1643–1644, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [OYK+11].

Rovigatti:2015:CBP

[RŠRR15] Lorenzo Rovigatti, Petr Šulc, István Z. Reguly, and Flavio Romano. A comparison between parallelization approaches in molecular dynamics simulations on GPUs. *Journal of Computational Chemistry*, 36(1):1–8, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raychev:2018:CAS

[RSSG18] Deyan Raychev, Gotthard Seifert, Jens-Uwe Sommer, and Olga Guskova. A comparative analysis of symmetric diketopyrrolopyrrole-cored small conjugated molecules with aromatic flanks: From geometry to charge transport. *Journal of Computational Chemistry*, 39(30):2526–2538, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roberts:2013:DMD

[RTP+13] Victoria A. Roberts, Elaine E. Thompson, Michael E. Pique, Martin S. Perez, and L. F. Ten Eyck. DOT2: Macromolecular docking with improved biophysical models. *Journal of Computational Chemistry*, 34(20):1743–1758, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Real:2013:FIA

[RTS+13] Florent Réal, Michael Trumm, Bernd Schimmelpfennig, Michel Masella, and Valérie Vallet. Further insights in the ability of classical nonadditive potentials to model actinide ion–water interactions. *Journal of Computational Chemistry*, 34(9):707–719, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ruiz:2011:ECC

[Rui11] Eliseo Ruiz. Exchange coupling constants using density functional theory: Long-range corrected functionals. *Journal of Computational Chemistry*, 32(9):1998–2004, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Randic:2012:CCC

[RVB+12] Milan Randić, Damir Vukičević, Alexandru T. Balaban, Marjan Vračko, and Dejan Plavšić. Conjugated circuits currents in hexabenzocoronene and its derivatives formed by joining proximal carbons. *Journal of Computational Chemistry*, 33 (11):1111–1122, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rey-Villaverde:2013:HAT

[RVCFF13] Ringo Rey-Villaverde, Hubert Cybulski, Jesús R. Flores, and Berta Fernández. A high-accuracy theoretical study of the CH_nP systems $n = 1$–3. *Journal of Computational Chemistry*, 34(23):2020–2031, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rodrigues:2016:UPU

[RVdMB16] Gessenildo Pereira Rodrigues, Elizete Ventura, Silmar Andrade do Monte, and Mario Barbatti. UV-photoexcitation and ultrafast dynamics of HCFC-132b (CF_2 $ClCH_2$ Cl). *Journal of Computational Chemistry*, 37(7):675–683, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rashid:2011:GKV

[RvL11] Zahid Rashid and Joop H. van Lenthe. Generation of Kekulé valence structures and the corresponding valence bond wave function. *Journal of Computational Chemistry*, 32(4):696–708, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Real:2019:IDS

[RVM19] Florent Réal, Valérie Vallet, and Michel Masella. Improving the description of solvent pairwise interactions using local solute/solvent three-body functions. The case of halides and carboxylates in aqueous environment. *Journal of Computational Chemistry*, 40(11):1209–1218, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roumen:2011:ALB

[RVP+11] Luc Roumen, Bram Van Hoof, Koen Pieterse, Peter A. J. Hilbers, Erica M. G. Custers, Ralf Plate, Marcel De Gooyer, Ilona P. E. Beugels, Judith M. A. Emmen, Dirk Leysen, Jos

F. M. Smits, Harry C. J. Ottenheijm, and J. J. Rob Hermans. Application of a ligand-based theoretical approach to derive conversion paths and ligand conformations in CYP11B2-mediated aldosterone formation. *Journal of Computational Chemistry*, 32(11):2441–2448, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rogan:2013:SFM

[RVVK13] José Rogan, Alejandro Varas, Juan Alejandro Valdivia, and Miguel Kiwi. A strategy to find minimal energy nanocluster structures. *Journal of Computational Chemistry*, 34(29): 2548–2556, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ren:2013:EEG

[RWR+13] Yi Ren, Xi-Guang Wei, Si-Jia Ren, Kai-Chung Lau, Ning-Bew Wong, and Wai-Kee Li. The α-effect exhibited in gas-phase S_N2@N and S_N2@C reactions. *Journal of Computational Chemistry*, 34(23):1997–2005, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reif:2016:RAC

[RZ16] Maria M. Reif and Martin Zacharias. Rapid approximate calculation of water binding free energies in the whole hydration domain of (bio)macromolecules. *Journal of Computational Chemistry*, 37(18):1711–1724, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rao:2013:NPL

[RZG+13] Li Rao, Igor Ying Zhang, Wenping Guo, Li Feng, Eric Meggers, and Xin Xu. Nonfitting protein–ligand interaction scoring function based on first-principles theoretical chemistry methods: Development and application on kinase inhibitors. *Journal of Computational Chemistry*, 34(19):1636–1646, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sattelle:2010:LMW

[SA10] Benedict M. Sattelle and Andrew Almond. Less is more when simulating unsulfated glycosaminoglycan 3D-structure: Comparison of GLYCAM06/TIP3P, PM3-CARB1/TIP3P, and SCC-DFTB-D/TIP3P predictions with experiment. *Journal of Computational Chemistry*, 31(16):2932–2947, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Swetnam:2011:IWL

[SA11] Adam D. Swetnam and Michael P. Allen. Improving the Wang–Landau algorithm for polymers and proteins. *Journal of Computational Chemistry*, 32(5):816–821, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schumann:2013:SES

[SA13] Marcel Schumann and Roger S. Armen. Systematic and efficient side chain optimization for molecular docking using a cheapest-path procedure. *Journal of Computational Chemistry*, 34(14):1258–1269, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spivak:2014:ICM

[SACdG14] Mariano Spivak, Celestino Angeli, Carmen J. Calzado, and Coen de Graaf. Improving the calculation of magnetic coupling constants in MRPT methods. *Journal of Computational Chemistry*, 35(23):1665–1671, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scemama:2016:QMC

[SAGC16] Anthony Scemama, Thomas Applencourt, Emmanuel Giner, and Michel Caffarel. Quantum Monte Carlo with very large multideterminant wavefunctions. *Journal of Computational Chemistry*, 37(20):1866–1875, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahni:2018:GST

[Sah18] Viraht Sahni. Generalization of the Schrödinger theory of electrons. *Journal of Computational Chemistry*, 39(18):1083–1089, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakata:2018:FCD

[Sak18] Ken Sakata. Force constant decomposition for pentacoordinated $X\mathrm{H}_3\mathrm{Cl}_2^-$ (X = C, Si, Ge) structures. *Journal of Computational Chemistry*, 39(20):1544–1550, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez:2017:RTC

[Sán17] Hernán R. Sánchez. Revisiting the thermochemistry of chlorine fluorides. *Journal of Computational Chemistry*, 38(22): 1930–1940, August 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szklarczyk:2015:PCG

[SAvG15] Oliwia M. Szklarczyk, Eirini Arvaniti, and Wilfred F. van Gunsteren. Polarizable coarse-grained models for molecular dynamics simulation of liquid cyclohexane. *Journal of Computational Chemistry*, 36(17):1311–1321, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sax:2012:LMO

[Sax12] Alexander F. Sax. Localization of molecular orbitals on fragments. *Journal of Computational Chemistry*, 33(17):1495–1510, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salehzadeh:2010:TSS

[SB10] Sadegh Salehzadeh and Mehdi Bayat. Theoretical studies on the structure and protonation of Cu(II) complexes of a series of tripodal aliphatic tetraamines: Good correlations with the experimental data. *Journal of Computational Chemistry*, 31(13):2371–2380, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silva:2011:HFO

[SB11] Alexander M. Silva and Itamar Borges Jr. How to find an optimum cluster size through topological site properties: MoS_x model clusters. *Journal of Computational Chemistry*, 32(10): 2186–2194, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stepanek:2013:CMC

[ŠB13] Petr Štěpánek and Petr Bouř. Computation of magnetic circular dichroism by sum-over-states summations. *Journal of Computational Chemistry*, 34(18):1531–1539, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Soydas:2014:AOO

[SB14] Emine Soydaş and Uğur Bozkaya. Assessment of the orbital-optimized coupled-electron pair theory for thermochemistry and kinetics: Improving on CCSD and CEPA(1). *Journal of Computational Chemistry*, 35(14):1073–1081, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stepanek:2015:OIS

[ŠB15] Petr Štěpánek and Petr Bouř. Origin-independent sum over states simulations of magnetic and electronic circular dichroism spectra via the localized orbital/local origin method. *Journal of Computational Chemistry*, 36(10):723–730, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shoaf:2018:TBA

[SB18] Ashley L. Shoaf and Craig A. Bayse. Trigger bond analysis of nitroaromatic energetic materials using Wiberg bond indices. *Journal of Computational Chemistry*, 39(19):1236–1248, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:2019:DAC

[SB19] Tejender Singh and Prasad V. Bharatam. Donor→ acceptor coordination interactions in 1,3-bis(NHC)triazenyl cations: an electronic structure analysis. *Journal of Computational Chemistry*, 40(25):2207–2215, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sedeh:2010:SIM

[SBB10] Reza Sharifi Sedeh, Mark Bathe, and Klaus-Jürgen Bathe. The subspace iteration method in protein normal mode analysis. *Journal of Computational Chemistry*, 31(1):66–74, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simpson:2011:EIC

[SBC+11] Darren J. Simpson, Thomas Bredow, Anand P. Chandra, Giuseppe P. Cavallaro, and Andrea R. Gerson. The effect of iron and copper impurities on the wettability of sphalerite (110) surface. *Journal of Computational Chemistry*, 32(9):

2022–2030, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sebesta:2017:IMC

[ŠBD+17] Filip Šebesta, Mateusz Z. Brela, Silvia Diaz, Sebastian Miranda, Jane S. Murray, Soledad Gutiérrez-Oliva, Alejandro Toro-Labbé, Artur Michalak, and Jaroslav V. Burda. The influence of the metal cations and microhydration on the reaction trajectory of the N_3O_2 thymine proton transfer: Quantum mechanical study. *Journal of Computational Chemistry*, 38(31):2680–2692, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schacht:2018:AOF

[SBGP18] Julia Schacht, Johannes Horst Budau, Nicola Gaston, and Beate Paulus. Aluminum oxo-fluoride clusters: a first principle investigation of stability, synthetic considerations, and the interaction with water. *Journal of Computational Chemistry*, 39(19):1208–1214, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spill:2013:CRE

[SBN13a] Yannick G. Spill, Guillaume Bouvier, and Michael Nilges. A convective replica-exchange method for sampling new energy basins. *Journal of Computational Chemistry*, 34(2):132–140, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [SBN13b].

Spill:2013:ECR

[SBN13b] Yannick G. Spill, Guillaume Bouvier, and Michael Nilges. Erratum: A convective replica-exchange method for sampling new energy basins. *Journal of Computational Chemistry*, 34 (18):1609, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SBN13a].

Saha:2013:HPD

[SBR13] Soumen Saha, Rituparna Bhattacharjee, and Ram Kinkar Roy. Hardness potential derivatives and their relation to Fukui indices. *Journal of Computational Chemistry*, 34(8):662–672, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sesmero:2017:MSD

[SBT17] Ester Sesmero, Jodian A. Brown, and Ian F. Thorpe. Molecular simulations to delineate functional conformational transitions in the HCV polymerase. *Journal of Computational Chemistry*, 38(15):1125–1137, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmid:2010:GSS

[SBV10] Nathan Schmid, Mathias Bötschi, and Wilfred F. Van Gunsteren. A GPU solvent–solvent interaction calculation accelerator for biomolecular simulations using the GROMOS software. *Journal of Computational Chemistry*, 31(8):1636–1643, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szklarczyk:2014:PEF

[SBvG14] Oliwia M. Szklarczyk, Stephan J. Bachmann, and Wilfred F. van Gunsteren. A polarizable empirical force field for molecular dynamics simulation of liquid hydrocarbons. *Journal of Computational Chemistry*, 35(10):789–801, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2012:IPM

[SBW12] Wenming Sun, Yuxiang Bu, and Yixuan Wang. Interaction and protection mechanism between li@C_{60} and nucleic acid bases (NABs): Performance of PM6-DH2 on noncovalent interaction of NABs-Li@C60. *Journal of Computational Chemistry*, 33(5):490–501, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sibaev:2015:SNU

[SC15] Marat Sibaev and Deborah L. Crittenden. Software news and updates: The PyPES library of high quality semi-global potential energy surfaces. *Journal of Computational Chemistry*, 36(29):2200–2207, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sode:2017:DFM

[SC17] Olaseni Sode and Jasmine N. Cherry. Development of a flexible-monomer two-body carbon dioxide potential and its application to clusters up to $(CO_2)_{13}$. *Journal of Computational Chemistry*, 38(32):2763–2774, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2018:NHS

[SC18a] Bikramjit Sharma and Amalendu Chandra. Nature of hydration shells of a polyoxy-anion with a large cationic centre: the case of iodate ion in water. *Journal of Computational Chemistry*, 39(19):1226–1235, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Soniya:2018:FEL

[SC18b] Kumari Soniya and Amalendu Chandra. Free energy landscapes of prototropic tautomerism in pyridoxal 5'-phosphate Schiff bases at the active site of an enzyme in aqueous medium. *Journal of Computational Chemistry*, 39(21):1629–1638, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scerri:2007:PTS

[Sce07] Eric R. Scerri. *The Periodic Table: Its Story and Its Significance*. Oxford University Press, Walton Street, Oxford OX2 6DP, UK, 2007. ISBN 0-19-530573-6. xxii + 346 pp. LCCN QD467 .S345 2007. URL http://www.loc.gov/catdir/enhancements/fy0635/2005037784-d.html; http://www.loc.gov/catdir/enhancements/fy0722/2005037784-b.html; http://www.loc.gov/catdir/toc/ecip065/2005037784.html.

Shiraogawa:2019:PPF

[SCF+19] Takafumi Shiraogawa, Gaelle Candel, Ryoichi Fukuda, Ilaria Ciofini, Carlo Adamo, Akimitsu Okamoto, and Masahiro Ehara. Photophysical properties of fluorescent imaging biological probes of nucleic acids: SAC-CI and TD-DFT study. *Journal of Computational Chemistry*, 40(1):127–134, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwarz:2010:BRP

[Sch10] W. H. Eugen Schwarz. Book review: *The Periodic Table: Its Story and Its Significance*, by Eric R. Scerri, ISBN-13: 978-0-19-530573-9. *Journal of Computational Chemistry*, 31(8):

1793–1794, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwabe:2012:AFT

[Sch12] Tobias Schwabe. Accurate and fast treatment of large molecular systems: Assessment of CEPA and pCCSD within the local pair natural orbital approximation. *Journal of Computational Chemistry*, 33(26):2067–2072, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmidling:2013:NSB

[Sch13] David Schmidling. A new set of bending T_d symmetry coordinates for MX_4 molecules. *Journal of Computational Chemistry*, 34(32):2771–2773, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scheiner:2018:CVM

[Sch18] Steve Scheiner. Comparison of various means of evaluating molecular electrostatic potentials for noncovalent interactions. *Journal of Computational Chemistry*, 39(9):500–510, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shupanov:2018:MPC

[SCK18] Ruslan Shupanov, Alexander Chertovich, and Pavel Kos. Micellar polymerization: Computer simulations by dissipative particle dynamics. *Journal of Computational Chemistry*, 39 (19):1275–1284, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez:2015:NQM

[SCM+15] M. Luz Sánchez, José C. Corchado, M. Elena Martín, Ignacio Fdez. Galván, Rute Barata-Morgado, and Manuel A. Aguilar. A new QM/MM method oriented to the study of ionic liquids. *Journal of Computational Chemistry*, 36(25): 1893–1901, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2017:SDI

[SCMA+17] Bin Song, Nathaniel Charest, Herbert Alexander Morriss-Andrews, Valeria Molinero, and Joan-Emma Shea. Systematic derivation of implicit solvent models for the study of polymer collapse. *Journal of Computational Chemistry*, 38(16):1353–1361, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scemama:2013:QMC

[SCOJ13] Anthony Scemama, Michel Caffarel, Emmanuel Oseret, and William Jalby. Quantum Monte Carlo for large chemical systems: Implementing efficient strategies for petascale platforms and beyond. *Journal of Computational Chemistry*, 34(11): 938–951, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Starikova:2019:RDE

[SCSM19] Alyona A. Starikova, Maxim G. Chegerev, Andrey G. Starikov, and Vladimir I. Minkin. Rational design of electronically labile dinuclear Fe and Co complexes with 1,10-phenanthroline-5,6-diimine: a DFT study. *Journal of Computational Chemistry*, 40(26):2284–2292, October 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2013:EAC

[SCSW13] Jinshuai Song, Zhenhua Chen, Sason Shaik, and Wei Wu. An efficient algorithm for complete active space valence bond self-consistent field calculation. *Journal of Computational Chemistry*, 34(1):38–48, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Selvam:2011:MZI

[SCW11] Lalitha Selvam, Fang Fang Chen, and Feng Wang. Methylation of zebularine investigated using density functional theory calculations. *Journal of Computational Chemistry*, 32(10): 2077–2083, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Signorile:2016:RDF

[SDB+16] Matteo Signorile, Alessandro Damin, Francesca Bonino, Valentina Crocellà, Carlo Lamberti, and Silvia Bordiga. The role of dispersive forces determining the energetics of adsorption in Ti zeolites. *Journal of Computational Chemistry*, 37(30):2659–2666, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shi:2012:USA

[SDF12] Guosheng Shi, Yihong Ding, and Haiping Fang. Unexpectedly strong anion–π interactions on the graphene flakes. *Journal of Computational Chemistry*, 33(14):1328–1337, May 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schieschke:2017:CFD

[SDF+17] Nils Schieschke, Roberto Di Remigio, Luca Frediani, Johannes Heuser, and Sebastian Höfener. Combining frozen-density embedding with the conductor-like screening model using Lagrangian techniques for response properties. *Journal of Computational Chemistry*, 38(19):1693–1703, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schulz:2018:SHA

[SDIP18] Christine E. Schulz, Achintya Kumar Dutta, Róbert Izsák, and Dimitrios A. Pantazis. Systematic High-Accuracy Prediction of Electron Affinities for Biological Quinones. *Journal of Computational Chemistry*, 39(29):2439–2451, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suarez:2014:CSD

[SDL14] Dimas Suárez, Natalia Díaz, and Ramón López. A combined semiempirical and DFT computational protocol for studying bioorganometallic complexes: Application to molybdocene–cysteine complexes. *Journal of Computational Chemistry*, 35 (4):324–334, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sergentu:2016:SIA

[SDM+16] Dumitru-Claudiu Sergentu, Grégoire David, Gilles Montavon, Rémi Maurice, and Nicolas Galland. Scrutinizing "invisible" astatine: a challenge for modern density functionals. *Journal of Computational Chemistry*, 37(15):1345–1354, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suarez:2013:SNU

[SDMS13] Ernesto Suárez, Natalia Díaz, Jefferson Méndez, and Dimas Suárez. Software news and updates: CENCALC: a computational tool for conformational entropy calculations from molecular simulations. *Journal of Computational Chemistry*, 34(23):2041–2054, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shen:2017:ECC

[SDZ17] Hujun Shen, Mingsen Deng, and Yachao Zhang. Extension of CAVS coarse-grained model to phospholipid membranes: the importance of electrostatics. *Journal of Computational Chemistry*, 38(13):971–980, May 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shirazi:2014:AKM

[SE14] Mahdi Shirazi and Simon D. Elliott. Atomistic kinetic Monte Carlo study of atomic layer deposition derived from density functional theory. *Journal of Computational Chemistry*, 35 (3):244–259, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seal:2010:CRG

[Sea10] Prasenjit Seal. Carbondioxide rare-gas systems: Sensitivity of basis sets and double-hybrid density functionals. *Journal of Computational Chemistry*, 31(10):2001–2007, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shaghaghi:2016:SGA

[SEF+16] Hoora Shaghaghi, Hossein Pasha Ebrahimi, Fariba Fathi, Niloufar Bahrami Panah, Mehdi Jalali-Heravi, and Mohsen Tafazzoli. A simple graphical approach to predict local residue conformation using NMR chemical shifts and density functional theory. *Journal of Computational Chemistry*, 37(14): 1296–1305, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shiraogawa:2018:FED

[SEJ+18] Takafumi Shiraogawa, Masahiro Ehara, Sandro Jurinovich, Lorenzo Cupellini, and Benedetta Mennucci. Frenkel-exciton decomposition analysis of circular dichroism and circularly polarized luminescence for multichromophoric systems. *Journal of Computational Chemistry*, 39(16):931–935, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Solomentsev:2012:EEE

[SEM12] Gleb Y. Solomentsev, Niall J. English, and Damian A. Mooney. Effects of external electromagnetic fields on the conformational sampling of a short alanine peptide. *Journal of Computational Chemistry*, 33(9):917–923, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakuraba:2018:PEZ

[SF18] Shun Sakuraba and Ikuo Fukuda. Performance evaluation of the zero-multipole summation method in modern molecular dynamics software. *Journal of Computational Chemistry*, 39 (20):1551–1560, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schleder:2017:DCB

[SFA17] Gabriel R. Schleder, Adalberto Fazzio, and Jeverson T. Arantes. Dynamic covalent bond from first principles: Diarylbibenzofuranone structural, electronic, and oxidation studies. *Journal of Computational Chemistry*, 38(31):2675–2679, December 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Starek:2017:GEV

[SFBT17] Greg Starek, J. Alfredo Freites, Simon Bernèche, and Douglas J. Tobias. Gating energetics of a voltage-dependent K^+ channel pore domain. *Journal of Computational Chemistry*, 38(16):1472–1478, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez-Flores:2014:PAE

[SFCCK+14] Eric Iván Sánchez-Flores, Rodrigo Chávez-Calvillo, Todd A. Keith, Gabriel Cuevas, Tomás Rocha-Rinza, and Fernando Cortés-Guzmán. Properties of atoms in electronically excited molecules within the formalism of TDDFT. *Journal of Computational Chemistry*, 35(10):820–828, April 15, 2014. CO-

DEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [SFCCK+15].

Sanchez-Flores:2015:EPA

[SFCCK+15] Eric Iván Sánchez-Flores, Rodrigo Chávez-Calvillo, Todd A. Keith, Gabriel Cuevas, Tomás Rocha-Rinza, and Fernando Cortés-Guzmán. Erratum: Properties of atoms in electronically excited molecules within the formalism of TDDFT [J. Comput Chem. 2014, **35**, 820–828]. *Journal of Computational Chemistry*, 36(32):2429, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SFCCK+14].

Stehr:2016:CCM

[SFDE16] Vera Stehr, Reinhold F. Fink, Carsten Deibel, and Bernd Engels. Charge carrier mobilities in organic semiconductor crystals based on the spectral overlap. *Journal of Computational Chemistry*, 37(23):2146–2156, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schluns:2017:SNU

[SFG+17] Danny Schlüns, Mirko Franchini, Andreas W. Götz, Johannes Neugebauer, Christoph R. Jacob, and Lucas Visscher. Software news and updates: Analytical gradients for subsystem density functional theory within the Slater-function-based Amsterdam density functional program. *Journal of Computational Chemistry*, 38(4):238–249, February 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steinmann:2017:LEM

[SFLG+17] Stephan N. Steinmann, Paul Fleurat-Lessard, Andreas W. Götz, Carine Michel, Rodrigo Ferreira de Morais, and Philippe Sautet. Letters to the Editor: Molecular mechanics models for the image charge, a comment on "Including image charge effects in the molecular dynamics simulations of molecules on metal surfaces". *Journal of Computational Chemistry*, 38(24):2127–2129, September 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See reply [Cor17].

San-Fabian:2014:CAR

[SFM14] Emilio San-Fabián and Federico Moscardó. Cyclobutadiene automerization and rotation of ethylene: Energetics of the barriers by using spin-polarized wave functions. *Journal of Computational Chemistry*, 35(18):1356–1363, July 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salvadori:2018:DCB

[SFM+18] Andrea Salvadori, Marco Fusè, Giordano Mancini, Sergio Rampino, and Vincenzo Barone. Diving into chemical bonding: an immersive analysis of the electron charge rearrangement through virtual reality. *Journal of Computational Chemistry*, 39(31):2607–2617, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seeber:2011:WUF

[SFR+11] Michele Seeber, Angelo Felline, Francesco Raimondi, Stefanie Muff, Ran Friedman, Francesco Rao, Amedeo Caflisch, and Francesca Fanelli. Wordom: a user-friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. *Journal of Computational Chemistry*, 32(6):1183–1194, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scott:2010:SLD

[SG10a] Gregory Scott and Martin Gruebele. Solving the low dimensional Smoluchowski equation with a singular value basis set. *Journal of Computational Chemistry*, 31(13):2428–2433, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sen:2010:WMN

[SG10b] Anik Sen and Bishwajit Ganguly. What is the minimum number of water molecules required to dissolve a potassium chloride molecule? *Journal of Computational Chemistry*, 31(16): 2948–2954, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sure:2013:CSB

[SG13] Rebecca Sure and Stefan Grimme. Corrected small basis set Hartree–Fock method for large systems. *Journal of Computational Chemistry*, 34(19):1672–1685, July 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez-Garcia:2010:QMS

[SGDT10] Elsa Sanchez-Garcia, Markus Doerr, and Walter Thiel. QM/MM study of the absorption spectra of DsRed.M1 chromophores. *Journal of Computational Chemistry*, 31(8):1603–1612, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sviatenko:2016:SEP

[SGH+16] Liudmyla K. Sviatenko, Leonid Gorb, Frances C. Hill, Danuta Leszczynska, and Jerzy Leszczynski. Structure and electrochemical properties for complexes of nitrocompounds with inorganic ions: a theoretical approach. *Journal of Computational Chemistry*, 37(13):1206–1213, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sviatenko:2013:TSI

[SGHL13] Liudmyla K. Sviatenko, Leonid Gorb, Frances C. Hill, and Jerzy Leszczynski. Theoretical study of ionization and one-electron oxidation potentials of N-heterocyclic compounds. *Journal of Computational Chemistry*, 34(13):1094–1100, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simonson:2013:CPD

[SGM+13] Thomas Simonson, Thomas Gaillard, David Mignon, Marcel Schmidt am Busch, Anne Lopes, Najette Amara, Savvas Polydorides, Audrey Sedano, Karen Druart, and Georgios Archontis. Computational protein design: the Proteus software and selected applications. *Journal of Computational Chemistry*, 34(28):2472–2484, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smith:2018:MSS

[SGP18] Marisa E. Smith, N. J. B. Green, and S. M. Pimblott. Methods for the Simulation of the Slowing of Low-Energy Electrons in Water. *Journal of Computational Chemistry*, 39(26):2217–2225, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sancho-Garcia:2017:DRU

[SGPJS+17] Juan Carlos Sancho-García, Ángel José Pérez-Jiménez, Marika Savarese, Éric Brémond, and Carlo Adamo. Determining the role of the underlying orbital-dependence of PBE0-DH and PBE-QIDH double-hybrid density functionals. *Journal of Computational Chemistry*, 38(17):1509–1514, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shernyukov:2016:NBB

[SGS+16] Andrey V. Shernyukov, Alexander M. Genaev, George E. Salnikov, Henry S. Rzepa, and Vyacheslav G. Shubin. Noncatalytic bromination of benzene: a combined computational and experimental study. *Journal of Computational Chemistry*, 37 (2):210–225, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szefczyk:2017:ESM

[SGWA17] Borys Szefczyk, Dawid Grabarek, Elżbieta Walczak, and Tadeusz Andruniów. Excited-state minima and emission energies of retinal chromophore analogues: Performance of CASSCF and CC2 methods as compared with CASPT2. *Journal of Computational Chemistry*, 38(20):1799–1810, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sieradzan:2018:NPN

[SGY+18] Adam K. Sieradzan, Artur Gieldoń, Yanping Yin, Yi He, Harold A. Scheraga, and Adam Liwo. A new protein nucleic-acid coarse-grained force field based on the UNRES and NARES-2P force fields. *Journal of Computational Chemistry*, 39(28):2360–2370, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sheppard:2011:PWN

[SH11a] Daniel Sheppard and Graeme Henkelman. Paths to which the nudged elastic band converges. *Journal of Computational Chemistry*, 32(8):1769–1771, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See reply [QB11].

Smiatek:2011:CFE

[SH11b] Jens Smiatek and Andreas Heuer. Calculation of free energy landscapes: a histogram reweighted metadynamics approach. *Journal of Computational Chemistry*, 32(10):2084–2096, July

30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shukla:2014:PWD

[SH14] Manoj K. Shukla and Frances Hill. Plane-wave density functional theory investigation of adsorption of 2,4,6-trinitrotoluene on Al-hydroxylated (0001) surface of (4×4) α-alumina. *Journal of Computational Chemistry*, 35(27):1977–1985, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Santiago:2015:NDF

[SH15] Régis Tadeu Santiago and Roberto Luiz Andrade Haiduke. New density functional parameterizations to accurate calculations of electric field gradient variations among compounds. *Journal of Computational Chemistry*, 36(28):2125–2130, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shil:2018:PRS

[SH18a] Suranjan Shil and Carmen Herrmann. Performance of range-separated hybrid exchange-correlation functionals for the calculation of magnetic exchange coupling constants of organic diradicals. *Journal of Computational Chemistry*, 39(13):780–787, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steenbock:2018:TAA

[SH18b] Torben Steenbock and Carmen Herrmann. Toward an automated analysis of exchange pathways in spin-coupled systems. *Journal of Computational Chemistry*, 39(2):81–92, January 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2019:ALR

[SH19a] Jong-Won Song and Kimihiko Hirao. Accelerated long-range corrected exchange functional using a two-Gaussian operator combined with one-parameter progressive correlation functional [LC-BOP(2Gau)]. *Journal of Computational Chemistry*, 40(1):105–112, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Svatunek:2019:APT

[SH19b] Dennis Svatunek and Kendall N. Houk. autoDIAS: a python tool for an automated distortion/interaction activation strain analysis. *Journal of Computational Chemistry*, 40(28):2509–2515, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suess:2017:QCC

[SHB17] Christian J. Suess, Jonathan D. Hirst, and Nicholas A. Besley. Quantum chemical calculations of tryptophan heme electron and excitation energy transfer rates in myoglobin. *Journal of Computational Chemistry*, 38(17):1495–1502, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sherman:2012:SNU

[She12] William B. Sherman. Software news and updates: HolT Hunter: Software for identifying and characterizing low-strain DNA Holliday triangles. *Journal of Computational Chemistry*, 33(15):1393–1405, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sergiievskyi:2011:MSR

[SHF11] Volodymyr P. Sergiievskyi, Wolfgang Hackbusch, and Maxim V. Fedorov. Multigrid solver for the reference interaction site model of molecular liquids theory. *Journal of Computational Chemistry*, 32(9):1982–1992, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sega:2018:PPP

[SHFJ18] Marcello Sega, György Hantal, Balázs Fábián, and Pál Jedlovszky. Pytim: a Python package for the interfacial analysis of molecular simulations. *Journal of Computational Chemistry*, 39(25):2118–2125, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shin:2011:LPL

[SHL+11] Woong-Hee Shin, Lim Heo, Juyong Lee, Junsu Ko, Chaok Seok, and Jooyoung Lee. LigDockCSA: Protein–ligand docking using conformational space annealing. *Journal of Computational Chemistry*, 32(15):3226–3232, November 30, 2011.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smith:2013:CSE

[SHL+13] Shelley A. Smith, Karen E. Hand, Melissa L. Love, Glake Hill, and David H. Magers. Conventional strain energies of azetidine and phosphetane: Can density functional theory yield reliable results? *Journal of Computational Chemistry*, 34(7): 558–565, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwalbe:2018:FLO

[SHL+18] Sebastian Schwalbe, Torsten Hahn, Simon Liebing, Kai Trepte, and Jens Kortus. Fermi–Löwdin orbital self-interaction corrected density functional theory: Ionization potentials and enthalpies of formation. *Journal of Computational Chemistry*, 39(29):2463–2471, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shang:2019:MPS

[SHL19] Cheng Shang, Si-Da Huang, and Zhi-Pan Liu. Massively parallelization strategy for material simulation using high-dimensional neural network potential. *Journal of Computational Chemistry*, 40(10):1091–1096, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakae:2011:PSP

[SHMO11] Yoshitake Sakae, Tomoyuki Hiroyasu, Mitsunori Miki, and Yuko Okamoto. Protein structure predictions by parallel simulated annealing molecular dynamics using genetic crossover. *Journal of Computational Chemistry*, 32(7):1353–1360, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sieradzan:2015:SNU

[Sie15] Adam K. Sieradzan. Software news and updates: Introduction of periodic boundary conditions into UNRES force field. *Journal of Computational Chemistry*, 36(12):940–946, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Siegbahn:2018:TCS

[Sie18] Per E. M. Siegbahn. Is there computational support for an unprotonated carbon in the E_4 state of nitrogenase? *Journal of Computational Chemistry*, 39(12):743–747, May 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sviatenko:2011:TRC

[SIG+11] Liudmila Sviatenko, Olexandr Isayev, Leonid Gorb, Frances Hill, and Jerzy Leszczynski. Toward robust computational electrochemical predicting the environmental fate of organic pollutants. *Journal of Computational Chemistry*, 32(10): 2195–2203, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sviatenko:2015:ROP

[SIG+15] Liudmyla K. Sviatenko, Olexandr Isayev, Leonid Gorb, Frances C. Hill, Danuta Leszczynska, and Jerzy Leszczynski. Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those produced when adsorbed on a silica surface? A DFT M05-2X computational study. *Journal of Computational Chemistry*, 36(14):1029–1035, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shaytan:2010:FEP

[SISK10] Alexey K. Shaytan, Victor A. Ivanov, Konstantin V. Shaitan, and Alexei R. Khokhlov. Free energy profiles of amino acid side chain analogs near water-vapor interface obtained via MD simulations. *Journal of Computational Chemistry*, 31(1):204–216, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:2018:IGS

[SIT18] Raman K. Singh, Takeshi Iwasa, and Tetsuya Taketsugu. Insights into geometries, stabilities, electronic structures, reactivity descriptors, and magnetic properties of bimetallic Ni_m Cu_{n-m} ($m = 1, 2$; $n = 3$–13) clusters: Comparison with pure copper clusters. *Journal of Computational Chemistry*, 39(23): 1878–1889, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2016:ETI

[SJ16] Pin-Chih Su and Michael E. Johnson. Evaluating thermodynamic integration performance of the new Amber molecular dynamics package and assess potential halogen bonds of enoyl-ACP reductase (FabI) benzimidazole inhibitors. *Journal of Computational Chemistry*, 37(9):836–847, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sieradzan:2017:SNU

[SJ17] Adam K. Sieradzan and Rafał Jakubowski. Software news and updates: Introduction of steered molecular dynamics into UNRES coarse-grained simulations package. *Journal of Computational Chemistry*, 38(8):553–562, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steinbrecher:2011:SCP

[SJC11] Thomas Steinbrecher, InSuk Joung, and David A. Case. Soft-core potentials in thermodynamic integration: Comparing one- and two-step transformations. *Journal of Computational Chemistry*, 32(15):3253–3263, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shao:2011:TSS

[SJD11] Chang-Bin Shao, Lin Jin, and Yi-Hong Ding. A theoretical survey on the structures, energetics, and isomerization pathways of the B_5O radical. *Journal of Computational Chemistry*, 32(5):771–777, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez:2014:QMS

[SJD14] Leslie Sánchez, Gonzalo A. Jaña, and Eduardo J. Delgado. A QM/MM study on the reaction pathway leading to 2-Aceto-2-hydroxybutyrate in the catalytic cycle of AHAS. *Journal of Computational Chemistry*, 35(6):488–494, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stoliaroff:2018:PEU

[SJL18] Adrien Stoliaroff, Stéphane Jobic, and Camille Latouche. PyDEF 2.0: An easy to use post-treatment software for publishable charts featuring a graphical user interface. *Journal* *of Computational Chemistry*, 39(26):2251–2261, October 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sannyal:2019:TEP

[SJSS19] Arindam Sannyal, Joonkyung Jang, Md. Shajahan, and Joyanta K. Saha. Thermal effect on positive patterned self-assembled monolayer grown from a droplet of alkanethiol. *Journal of Computational Chemistry*, 40(30):2636–2642, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schlund:2010:PTE

[SJWE10] Sebastian Schlund, Eline M. Basílio Janke, Klaus Weisz, and Bernd Engels. Predicting the tautomeric equilibrium of acetylacetone in solution. I. The right answer for the wrong reason? *Journal of Computational Chemistry*, 31(4):665–670, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2015:ODO

[SJZ+15] Qi Song, Zhenyi Jiang, Zhiyong Zhang, Yuqing Hou, and Xiaodong Zhang. From orientation disordered to ordered — an ab initio simulation on ammonia borane phase transition within van der Waals corrections. *Journal of Computational Chemistry*, 36(1):22–32, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szarek:2011:MED

[SK11] Paweł Szarek and Ludwik Komorowski. Modeling the electron density kernels. *Journal of Computational Chemistry*, 32(8): 1721–1724, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2012:CPV

[SK12] Ity Sharma and George A. Kaminski. Calculating pK_a values for substituted phenols and hydration energies for other compounds with the first-order fuzzy-border continuum solvation model. *Journal of Computational Chemistry*, 33(30): 2388–2399, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stachowicz:2013:BDM

[SK13] Anna Stachowicz and Jacek Korchowiec. Bond detectors for molecular dynamics simulations, Part I: Hydrogen bonds. *Journal of Computational Chemistry*, 34(26):2261–2269, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakalli:2015:PPS

[SK15a] Ilkay Sakalli and Ernst-Walter Knapp. pK_A in proteins solving the Poisson–Boltzmann equation with finite elements. *Journal of Computational Chemistry*, 36(29):2147–2157, November 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schultz:2015:SNU

[SK15b] Andrew J. Schultz and David A. Kofke. Software news and updates: Etomica: an object-oriented framework for molecular simulation. *Journal of Computational Chemistry*, 36(8): 573–583, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2017:UPP

[SK17] Ity Sharma and George A. Kaminski. Using polarizable POSSIM force field and fuzzy-border continuum solvent model to calculate pK_a shifts of protein residues. *Journal of Computational Chemistry*, 38(2):65–80, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silanteva:2018:RDE

[SK18] Irina Silanteva and Andrei V. Komolkin. Representation of DNA environment: Spiral staircase distribution function. *Journal of Computational Chemistry*, 39(27):2300–2306, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmidt:2019:WMP

[SKA19] Burkhard Schmidt, Rupert Klein, and Leonardo Cancissu Araujo. WavePacket: a Matlab package for numerical quantum dynamics. III. Quantum-classical simulations and surface hopping trajectories. *Journal of Computational Chemistry*, 40(30):2677–2688, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szatylowicz:2013:CSP

[SKGB13] Halina Szatyłowicz, Tadeusz M. Krygowski, Célia Fonseca Guerra, and F. Matthias Bickelhaupt. Complexes of 4-substituted phenolates with HF and HCN: Energy decomposition and electronic structure analyses of hydrogen bonding. *Journal of Computational Chemistry*, 34(8):696–705, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sethurajan:2019:BUQ

[SKGP19] Athinthra Sethurajan, Sergey Krachkovskiy, Gillian Goward, and Bartosz Protas. Bayesian uncertainty quantification in inverse modeling of electrochemical systems. *Journal of Computational Chemistry*, 40(5):740–752, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shin:2013:GPL

[SKKS13] Woong-Hee Shin, Jae-Kwan Kim, Deok-Soo Kim, and Chaok Seok. GalaxyDock2: Protein–ligand docking using beta-complex and global optimization. *Journal of Computational Chemistry*, 34(30):2647–2656, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Standara:2013:NCS

[SKMS13] Stanislav Standara, Petr Kulhánek, Radek Marek, and Michal Straka. ^{129}Xe NMR chemical shift in Xe@C_{60} calculated at experimental conditions: Essential role of the relativity, dynamics, and explicit solvent. *Journal of Computational Chemistry*, 34(22):1890–1898, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2011:TSC

[SKTT11] Keju Sun, Masanori Kohyama, Shingo Tanaka, and Seiji Takeda. A theoretical study of CO adsorption on gold by Hückel theory and density functional theory calculations. *Journal of Computational Chemistry*, 32(15):3276–3282, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sumimoto:2011:TSM

[SKY+11] Michinori Sumimoto, Yukio Kawashima, Daisuke Yokogawa, Kenji Hori, and Hitoshi Fujimoto. Theoretical study on the molecular structures of X-, α-, and β-types of lithium phthalocyanine dimer. *Journal of Computational Chemistry*, 32(14): 3062–3067, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Safi:2010:RDE

[SL10] Maria Safi and Ryan H. Lilien. Restricted dead-end elimination: Protein redesign with a bounded number of residue mutations. *Journal of Computational Chemistry*, 31(6):1207–1215, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Siegbahn:2017:CSC

[SL17] Per E. M. Siegbahn and Xichen Li. Cluster size convergence for the energetics of the oxygen evolving complex in PSII. *Journal of Computational Chemistry*, 38(25):2157–2160, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Surakhot:2017:TRR

[SLC+17] Yaowarat Surakhot, Viktor Laszlo, Chirawat Chitpakdee, Vinich Promarak, Taweesak Sudyoadsuk, Nawee Kungwan, Tim Kowalczyk, Stephan Irle, and Siriporn Jungsuttiwong. Theoretical rationalization for reduced charge recombination in bulky carbazole-based sensitizers in solar cells. *Journal of Computational Chemistry*, 38(12):901–909, May 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stenrup:2015:CNG

[SLG15] Michael Stenrup, Roland Lindh, and Ignacio Fdez. Galván. Constrained numerical gradients and composite gradients: Practical tools for geometry optimization and potential energy surface navigation. *Journal of Computational Chemistry*, 36(22):1698–1708, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2009:ETS

[SLHW09] Xinli Song, Jicun Li, Hua Hou, and Baoshan Wang. Extensive theoretical studies of a new energetic material: Tetrazino-tetrazine-tetraoxide (TTTO). *Journal of Computational Chemistry*, 30(12):1816–1820, September 2009. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [JW12].

Sladek:2012:ICS

[SLIB12] Vladimír Sládek, Vladimír Lukeš, Michal Ilčin, and Stanislav Biskupič. Ab initio calculation of structure and transport properties of He…X (X = Zn, Cd, Hg) van der Waals complexes. *Journal of Computational Chemistry*, 33(7):767–778, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2013:CMS

[SLLL13] Jen-Ping Su, Yung-Ting Lee, Shao-Yu Lu, and Jyh Shing Lin. Chemical mechanism of surface-enhanced Raman scattering spectrum of pyridine adsorbed on Ag cluster: Ab initio molecular dynamics approach. *Journal of Computational Chemistry*, 34(32):2806–2815, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Settels:2012:CES

[SLP+12] Volker Settels, Wenlan Liu, Jens Pflaum, Reinhold F. Fink, and Bernd Engels. Comparison of the electronic structure of different perylene-based dye-aggregates. *Journal of Computational Chemistry*, 33(18):1544–1553, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sala:2014:SET

[SLT14] Oliver Sala, Hans Peter Lüthi, and Antonio Togni. The solvent effect on two competing reaction mechanisms involving hypervalent iodine reagents (λ^3-iodanes): Facing the limit of the stationary quantum chemical approach. *Journal of Computational Chemistry*, 35(29):2122–2131, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sala:2015:DCR

[SLT+15] Oliver Sala, Hans Peter Lüthi, Antonio Togni, Marcella Iannuzzi, and Jürg Hutter. Dividing a complex reaction involving a hypervalent iodine reagent into three limiting mechanisms by ab initio molecular dynamics. *Journal of Computational Chemistry*, 36(11):785–794, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shen:2015:ACG

[SLX+15] Hujun Shen, Yan Li, Peijun Xu, Xiaofang Li, Huiying Chu, Dinglin Zhang, and Guohui Li. An anisotropic coarse-grained model based on Gay–Berne and electric multipole potentials and its application to simulate a DMPC bilayer in an implicit solvent model. *Journal of Computational Chemistry*, 36(15): 1103–1113, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sano:2010:MDC

[SLY+10] Eri Sano, Weihua Li, Hitomi Yuki, Xinli Liu, Tomomi Furihata, Kaoru Kobayashi, Kan Chiba, Saburo Neya, and Tyuji Hoshino. Mechanism of the decrease in catalytic activity of human cytochrome P450 2C9 polymorphic variants investigated by computational analysis. *Journal of Computational Chemistry*, 31(15):2746–2758, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2019:ABC

[SLY+19] Xin Sun, Xin Li, Jiong Yang, Jinyang Xi, Ryky Nelson, Christina Ertural, Richard Dronskowski, Weishu Liu, Gerald J. Snyder, David J. Singh, and Wenqing Zhang. Achieving band convergence by tuning the bonding ionicity in n-type Mg_3Sb_2. *Journal of Computational Chemistry*, 40(18): 1693–1700, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seetin:2011:ART

[SM11] Matthew G. Seetin and David H. Mathews. Automated RNA tertiary structure prediction from secondary structure and low-resolution restraints. *Journal of Computational Chemistry*, 32(10):2232–2244, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakuraba:2014:SNU

[SM14a] Shun Sakuraba and Nobuyuki Matubayasi. Software news and updates: Ermod: Fast and versatile computation software for solvation free energy with approximate theory of solutions. *Journal of Computational Chemistry*, 35(21):1592–1608, August 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Savelyev:2014:AAP

[SM14b] Alexey Savelyev and Alexander D. MacKerell Jr. All-atom polarizable force field for DNA based on the classical Drude oscillator model. *Journal of Computational Chemistry*, 35 (16):1219–1239, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stachiewicz:2015:CGM

[SM15] Anna Stachiewicz and Andrzej Molski. A coarse-grained MARTINI-like force field for DNA unzipping in nanopores. *Journal of Computational Chemistry*, 36(13):947–956, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salehzadeh:2016:NEC

[SM16a] Sadegh Salehzadeh and Farahnaz Maleki. New equation for calculating total interaction energy in one noncyclic ABC triad and new insights into cooperativity of noncovalent bonds. *Journal of Computational Chemistry*, 37(32):2799–2807, December 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stachiewicz:2016:DDD

[SM16b] Anna Stachiewicz and Andrzej Molski. Diffusive dynamics of DNA unzipping in a nanopore. *Journal of Computational Chemistry*, 37(5):467–476, February 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szczepaniak:2017:ARB

[SM17] Marek Szczepaniak and Jerzy Moc. Anomerization reaction of bare and microhydrated *d*-erythrose via explicitly correlated coupled cluster approach. Two water molecules are optimal. *Journal of Computational Chemistry*, 38(5):288–303, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stuart:2018:DII

[SM18] Duncan W. Stuart and Nicholas J. Mosey. Direct inversion of the iterative subspace with contracted planewave basis functions. *Journal of Computational Chemistry*, 39(23):1890–1901, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shibl:2018:WHN

[SMB18] Mohamed F. Shibl, Salvador Moncho, and Edward N. Brothers. What Happens Without Nickel? Cyclization Reactions of Ethylene with Ethanedithial and Related Molecules. *Journal of Computational Chemistry*, 39(18):1158–1167, July 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suresh:2018:NBS

[SMD18] Cherumuttathu H. Suresh, Neetha Mohan, and Therese Davis Della. A Noncovalent Binding Strategy to Capture Noble Gases, Hydrogen and Nitrogen. *Journal of Computational Chemistry*, 39(15):901–908, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sachse:2018:PAP

[SMDP18] Torsten Sachse, Todd J. Martínez, Benjamin Dietzek, and Martin Presselt. A program for automatically predicting supramolecular aggregates and its application to urea and porphin. *Journal of Computational Chemistry*, 39(13):763–772, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sheng:2011:CCU

[SMGB11] Xiao Wei Sheng, Lukasz Mentel, Oleg V. Gritsenko, and Evert Jan Baerends. Counterpoise correction is not useful for short and van der Waals distances but may be useful at long range. *Journal of Computational Chemistry*, 32(13):2896–2901, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shinagawa:2019:TSC

[SMiN+19] Chikashi Shinagawa, Yusuke Morikawa, Shin ichi Nishimura, Hiroshi Ushiyama, Atsuo Yamada, and Koichi Yamashita. A theoretical study on the charge and discharge states of Na-ion battery cathode material, $Na_1+x FePO_4F$. *Journal of Computational Chemistry*, 40(1):237–246, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sumi:2015:ESF

[SMM15a] Tomonari Sumi, Ayori Mitsutake, and Yutaka Maruyama. Erratum: "A solvation-free-energy functional: a reference-modified density functional formulation" [J. Comput. Chem. 2015, **36**, 1359–1369]. *Journal of Computational Chemistry*, 36(26):2009–2011, October 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SMM15b].

Sumi:2015:SFE

[SMM15b] Tomonari Sumi, Ayori Mitsutake, and Yutaka Maruyama. A solvation-free-energy functional: a reference-modified density functional formulation. *Journal of Computational Chemistry*, 36(18):1359–1369, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [SMM15a].

Suzuki:2017:MMT

[SMM17] Kimichi Suzuki, Keiji Morokuma, and Satoshi Maeda. Multistructural microiteration technique for geometry optimization and reaction path calculation in large systems. *Journal of Computational Chemistry*, 38(26):2213–2221, October 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sumi:2018:ARM

[SMM+18] Tomonari Sumi, Yutaka Maruyama, Ayori Mitsutake, Kenji Mochizuki, and Kenichiro Koga. Application of reference-modified density functional theory: Temperature and pressure dependences of solvation free energy. *Journal of Computational Chemistry*, 39(4):202–217, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sinha:2017:CEF

[SMP17a] Sudipta Kumar Sinha, Mohit Mehta, and Sandeep Patel. A charge equilibration formalism for treating charge transfer effects in MD simulations: Application to water clusters. *Journal of Computational Chemistry*, 38(16):1389–1409, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Snamina:2017:PAM

[SMP17b] Mateusz Snamina, Grzegorz Mazur, and Piotr Petelenz. Partial atomic multipoles for internally consistent microelectrostatic calculations. *Journal of Computational Chemistry*, 38 (28):2420–2429, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shah:2017:SNU

[SMRM+17] Jindal K. Shah, Eliseo Marin-Rimoldi, Ryan Gotchy Mullen, Brian P. Keene, Sandip Khan, Andrew S. Paluch, Neeraj Rai, Lucienne L. Romanielo, Thomas W. Rosch, Brian Yoo, and Edward J. Maginn. Software news and updates: Cassandra: an open source Monte Carlo package for molecular simulation. *Journal of Computational Chemistry*, 38(19):1727–1739, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Strumpfer:2010:CFE

[SN10] Johan Strümpfer and Kevin J. Naidoo. Computing free energy hypersurfaces for anisotropic intermolecular associations. *Journal of Computational Chemistry*, 31(2):308–316, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahoo:2015:PLP

[SN15] Sudhir K. Sahoo and Nisanth N. Nair. A potential with low point charges for pure siliceous zeolites. *Journal of Computational Chemistry*, 36(20):1562–1567, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahoo:2016:CGQ

[SN16a] Sudhir K. Sahoo and Nisanth N. Nair. CPMD/GULP QM/MM interface for modeling periodic solids: Implementation and its application in the study of Y-zeolite supported Rh_n

clusters. *Journal of Computational Chemistry*, 37(18):1657–1667, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seino:2016:IBE

[SN16b] Junji Seino and Hiromi Nakai. Informatics-based energy fitting scheme for correlation energy at complete basis set limit. *Journal of Computational Chemistry*, 37(25):2304–2315, September 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

SilvaLopez:2016:AAR

[SNDK16] Carlos Silva Lopez, Olalla Nieto Faza, Frank De Proft, and Antonios Kolocouris. Assessing the attractive/repulsive force balance in axial cyclohexane C–$H_{ax} \cdots Y_{ax}$ contacts: a combined computational analysis in monosubstituted cyclohexanes. *Journal of Computational Chemistry*, 37(30):2647–2658, November 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sekiya:2010:RCB

[SNKS10] Masahiro Sekiya, Takeshi Noro, Toshikatsu Koga, and Shiro L. Saito. Relativistic correlating basis sets for ${}_{57}$La and ${}_{89}$Ac. *Journal of Computational Chemistry*, 31(3):497–499, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Strobusch:2013:AHE

[SNS13] Daniel Strobusch, Mathias Nest, and Christoph Scheurer. The adaptive hierarchical expansion of the kinetic energy operator. *Journal of Computational Chemistry*, 34(14):1210–1217, May 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2016:SEC

[SNS16] Bhaskar Sharma, Y. Indra Neela, and G. Narahari Sastry. Structures and energetics of complexation of metal ions with ammonia, water, and benzene: a computational study. *Journal of Computational Chemistry*, 37(11):992–1004, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steiner:2011:CBF

[SOD+11] Denise Steiner, Chris Oostenbrink, François Diederich, Martina Zürcher, and Wilfred F. van Gunsteren. Calculation of binding free energies of inhibitors to plasmepsin II. *Journal of Computational Chemistry*, 32(9):1801–1812, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smeeton:2014:VEL

[SOJ14] Lewis C. Smeeton, Mark T. Oakley, and Roy L. Johnston. Visualizing energy landscapes with metric disconnectivity graphs. *Journal of Computational Chemistry*, 35(20):1481–1490, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shkurti:2013:ACG

[SOM+13] Ardita Shkurti, Mario Orsi, Enrico Macii, Elisa Ficarra, and Andrea Acquaviva. Acceleration of coarse grain molecular dynamics on GPU architectures. *Journal of Computational Chemistry*, 34(10):803–818, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steiner:2012:CRF

[SOvG12] Denise Steiner, Chris Oostenbrink, and Wilfred F. van Gunsteren. Calculation of the relative free energy of oxidation of azurin at pH 5 and pH 9. *Journal of Computational Chemistry*, 33(17):1467–1477, June 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shahrokh:2012:QMD

[SOYC12] Kiumars Shahrokh, Anita Orendt, Garold S. Yost, and Thomas E. Cheatham III. Quantum mechanically derived AMBER-compatible heme parameters for various states of the cytochrome P450 catalytic cycle. *Journal of Computational Chemistry*, 33(2):119–133, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schild:2013:MCR

[SP13] Axel Schild and Beate Paulus. Multireference calculations for ring inversion and double bond shifting in cyclooctatetraene. *Journal of Computational Chemistry*, 34(16):1393–1397, June

15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2011:SLR

[SPH11] Jong-Won Song, Daoling Peng, and Kimihiko Hirao. A semiempirical long-range corrected exchange correlation functional including a short-range Gaussian attenuation (LCgau-B97). *Journal of Computational Chemistry*, 32(15):3269–3275, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schnack-Petersen:2018:RDH

[SPHF+18] Anna Kristina Schnack-Petersen, Pi A. B. Haase, Rasmus Faber, Patricio F. Provasi, and Stephan P. A. Sauer. RPA(D) and HRPA(D): Two new models for calculations of NMR indirect nuclear spin-spin coupling constants. *Journal of Computational Chemistry*, 39(32):2647–2666, December 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sciortino:2018:PIM

[SPL+18] Giuseppe Sciortino, Jaime Rodríguez-Guerra Pedregal, Agustí Lledós, Eugenio Garribba, and Jean-Didier Maréchal. Prediction of the interaction of metallic moieties with proteins: an update for protein-ligand docking techniques. *Journal of Computational Chemistry*, 39(1):42–51, January 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suma:2019:TUF

[SPM+19] Antonio Suma, Erik Poppleton, Michael Matthies, Petr Sulc, Flavio Romano, Ard A. Louis, Jonathan P. K. Doye, Cristian Micheletti, and Lorenzo Rovigatti. TacoxDNA: a user-friendly web server for simulations of complex DNA structures, from single strands to origami. *Journal of Computational Chemistry*, 40(29):2586–2595, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Springborg:2010:BRC

[Spr10] Michael Springborg. Book review: *Computational Chemistry Workbook*, by Thomas Heine, Jan-Ole Joswig, and Achim Gelessus, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2009, 250 pp. ISBN-10 3-527-32442-9. *Journal of Computational Chemistry*, 31(4):895–896, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sousa:2013:CAP

[SPR+13] Sérgio F. Sousa, Gaspar R. P. Pinto, António J. M. Ribeiro, João T. S. Coimbra, Pedro A. Fernandes, and Maria João Ramos. Comparative analysis of the performance of commonly available density functionals in the determination of geometrical parameters for copper complexes. *Journal of Computational Chemistry*, 34(24):2079–2090, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sproviero:2018:INE

[Spr18] Eduardo M. Sproviero. Intramolecular natural energy decomposition analysis: Applications to the rational design of foldamers. *Journal of Computational Chemistry*, 39(20):1367–1386, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saha:2012:CSS

[SPS+12] Supriya Saha, Sougata Pal, Pranab Sarkar, A. L. Rosa, and Th. Frauenheim. A complete set of self-consistent charge density-functional tight-binding parametrization of zinc chalcogenides (ZnX; X = O, S, Se, and Te). *Journal of Computational Chemistry*, 33(12):1165–1178, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szeleszczuk:2018:CWP

[SPZP18a] Lukasz Szeleszczuk, Dariusz Maciej Pisklak, and Monika Zielińska-Pisklak. Can we predict the structure and stability of molecular crystals under increased pressure? First-principles study of glycine phase transitions. *Journal of Computational Chemistry*, 39(19):1300–1306, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szeleszczuk:2018:DCC

[SPZP18b] Lukasz Szeleszczuk, Dariusz Maciej Pisklak, and Monika Zielińska-Pisklak. Does the choice of the crystal structure influence the results of the periodic DFT calculations? A case of glycine alpha polymorph GIPAW NMR parameters computations. *Journal of Computational Chemistry*, 39(14):853–861, May 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szeleszczuk:2019:HDN

[SPZP19] Lukasz Szeleszczuk, Dariusz M. Pisklak, and Monika Zielińska-Pisklak. How does the NMR thermometer work? Application of combined quantum molecular dynamics and GIPAW calculations into the study of lead nitrate. *Journal of Computational Chemistry*, 40(6):811–819, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Strohecker:2010:QCI

[SR10] Traci Strohecker and Herschel Rabitz. Quantum control implemented as combinatorial optimization. *Journal of Computational Chemistry*, 31(1):151–153, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szalay:2011:FCD

[SR11] Zsófia Szalay and János Rohonczy. Fast calculation of DNMR spectra on CUDA-enabled graphics card. *Journal of Computational Chemistry*, 32(7):1262–1270, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:2018:SPI

[SR18] Krishna Kant Singh and Stephane Redon. Single-pass incremental force updates for adaptively restrained molecular dynamics. *Journal of Computational Chemistry*, 39(8):412–423, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stein:2019:APF

[SR19] Christopher J. Stein and Markus Reiher. autoCAS: A program for fully automated multiconfigurational calculations. *Journal of Computational Chemistry*, 40(25):2216–2226, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakkal:2017:PCB

[SRA17] Leon A. Sakkal, Kyle Z. Rajkowski, and Roger S. Armen. Prediction of consensus binding mode geometries for related chemical series of positive allosteric modulators of adenosine and muscarinic acetylcholine receptors. *Journal of Computational Chemistry*, 38(15):1209–1228, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Savarese:2017:CPT

[SRF+17] Marika Savarese, Umberto Raucci, Ryoichi Fukuda, Carlo Adamo, Masahiro Ehara, Nadia Rega, and Ilaria Ciofini. Comparing the performance of TD-DFT and SAC-CI methods in the description of excited states potential energy surfaces: an excited state proton transfer reaction as case study. *Journal of Computational Chemistry*, 38(14):1084–1092, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shyichuk:2015:SDC

[SRL+15] Andrii Shyichuk, Marcin Runowski, Stefan Lis, Jakub Kaczkowski, and Andrzej Jezierski. Semiempirical and DFT computations of the influence of Tb(III) dopant on unit cell dimensions of cerium(III) fluoride. *Journal of Computational Chemistry*, 36(3):193–199, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sengupta:2016:BBA

[SRR16] Arkajyoti Sengupta, Raghunath O. Ramabhadran, and Krishnan Raghavachari. Breaking a bottleneck: Accurate extrapolation to "gold standard" CCSD(T) energies for large open shell organic radicals at reduced computational cost. *Journal of Computational Chemistry*, 37(2):286–295, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smith:2014:SES

[SRS14] Phillip V. Smith, Marian W. Radny, and G. Ali Shah. Surface electronic structure calculations using the MBJLDA potential: Application to Si(111)2 $\times$ 1. *Journal of Computational Chemistry*, 35(16):1248–1254, June 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schapiro:2015:SHA

[SRSLO15] Igor Schapiro, Daniel Roca-Sanjuán, Roland Lindh, and Massimo Olivucci. A surface hopping algorithm for nonadiabatic minimum energy path calculations. *Journal of Computational*

Chemistry, 36(5):312–320, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Samsonyuk:2013:CSP

[SS13a] Andriy Samsonyuk and Christoph Scheurer. Configuration space partitioning and matrix buildup scaling for the vibrational configuration interaction method. *Journal of Computational Chemistry*, 34(1):27–37, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schutt:2013:SFT

[SS13b] Ole Schütt and Daniel Sebastiani. Spectroscopic fingerprints of toroidal nuclear quantum delocalization via ab initio path integral simulations. *Journal of Computational Chemistry*, 34 (10):827–835, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simonson:2013:SGM

[SS13c] Thomas Simonson and Priyadarshi Satpati. Simulating GTP:Mg and GDP:Mg with a simple force field: a structural and thermodynamic analysis. *Journal of Computational Chemistry*, 34(10):836–846, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scherrer:2016:MEL

[SS16a] Arne Scherrer and Daniel Sebastiani. Moment expansion of the linear density-density response function. *Journal of Computational Chemistry*, 37(7):665–674, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schroder:2016:EDA

[SS16b] Heiner Schröder and Tobias Schwabe. Efficient determination of accurate atomic polarizabilities for polarizeable embedding calculations. *Journal of Computational Chemistry*, 37(22): 2052–2059, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shi:2019:CSF

[SS19] Xuetao Shi and H. Bernhard Schlegel. Controlling the strong field fragmentation of $ClCHO^+$ using two laser pulses — an ab initio molecular dynamics simulation. *Journal of Computational Chemistry*, 40(1):200–205, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Szczepanik:2017:RLR

[SSA+17] Dariusz W. Szczepanik, Miquel Solà, Marcin Andrzejak, Barbara Pawełek, Justyna Dominikowska, Mercedes Kukułka, Karol Dyduch, Tadeusz M. Krygowski, and Halina Szatylowicz. The role of the long-range exchange corrections in the description of electron delocalization in aromatic species. *Journal of Computational Chemistry*, 38(18):1640–1654, July 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sushko:2010:QMM

[SSAS10] Maria L. Sushko, Peter V. Sushko, Igor V. Abarenkov, and Alexander L. Shluger. QM/MM method for metal–organic interfaces. *Journal of Computational Chemistry*, 31(16):2955–2966, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Swart:2011:IID

[SSB11] Marcel Swart, Miquel Solà, and F. Matthias Bickelhaupt. Inter- and intramolecular dispersion interactions. *Journal of Computational Chemistry*, 32(6):1117–1127, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See corrigendum [SSB13].

Swart:2013:CII

[SSB13] M. Swart, M. Solà, and F. M. Bickelhaupt. Corrigendum: Inter- and intramolecular dispersion interactions. *Journal of Computational Chemistry*, 34(27):2401–2402, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SSB11].

Smiga:2016:AKS

[ŚSB+16] Szymon Śmiga, Fabio Della Sala, Adam Buksztel, Ireneusz Grabowski, and Eduardo Fabiano. Accurate Kohn–Sham ionization potentials from scaled-opposite-spin second-order optimized effective potential methods. *Journal of Computational Chemistry*, 37(22):2081–2090, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Setzler:2014:SIG

[SSBW14] Julia Setzler, Carolin Seith, Martin Brieg, and Wolfgang Wenzel. SLIM: an improved generalized Born implicit membrane model. *Journal of Computational Chemistry*, 35(28):2027–2039, October 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Savchenkova:2019:MRC

[SSC+19] Anna S. Savchenkova, Alexander S. Semenikhin, Ivan V. Chechet, Sergey G. Matveev, Alexander A. Konnov, and Alexander M. Mebel. Mechanism and rate constants of the CH_2 + CH_2 CO reactions in triplet and singlet states: a theoretical study. *Journal of Computational Chemistry*, 40(2): 387–399, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:2019:TPN

[SSD19] Vijay Singh, Shigeyoshi Sakaki, and Milind M. Deshmukh. Theoretical prediction of Ni(I)-catalyst for hydrosilylation of pyridine and quinoline. *Journal of Computational Chemistry*, 40(24):2119–2130, September 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2015:EDA

[SSGS15] Bhaskar Sharma, Hemant Kumar Srivastava, Gaddamanugu Gayatri, and Garikapati Narahari Sastry. Energy decomposition analysis of cation–π, metal ion–lone pair, hydrogen bonded, charge-assisted hydrogen bonded, and π–π interactions. *Journal of Computational Chemistry*, 36(8):529–538, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2009:EAE

[SSMW09] Lingchun Song, Jinshuai Song, Yirong Mo, and Wei Wu. An efficient algorithm for energy gradients and orbital optimization in valence bond theory. *Journal of Computational Chemistry*, 30(3):399–406, February 2009. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [vLBBR12].

Shimamura:2019:IMD

[SSNT19] Kohei Shimamura, Fuyuki Shimojo, Aiichiro Nakano, and Shigenori Tanaka. Ab initio molecular dynamics study of prebiotic production processes of organic compounds at meteorite impacts on ocean. *Journal of Computational Chemistry*, 40(2):349–359, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakae:2019:ESM

[SSO19] Yoshitake Sakae, John E. Straub, and Yuko Okamoto. Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. *Journal of Computational Chemistry*, 40(2):475–481, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahu:2013:BAS

[SSP+13] Chandan Sahu, Kaushik Sen, Srimanta Pakhira, Bhaskar Mondal, and Abhijit K. Das. Binding affinity of substituted ureido-benzenesulfonamide ligands to the carbonic anhydrase receptor: a theoretical study of enzyme inhibition. *Journal of Computational Chemistry*, 34(22):1907–1916, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shakhno:2019:EIP

[SSP19a] Dzmitry V. Shakhno, Aleh V. Shakhno, and Eugene Paulechka. Efficient implementation of periodic boundary conditions in Monte Carlo simulation. *Journal of Computational Chemistry*, 40(5):734–739, February 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2019:PAE

[SSP+19b] Xiaobo Sun, Thomas M. Soini, Jordi Poater, Trevor A. Hamlin, and F. Matthias Bickelhaupt. PyFrag 2019-Automating the exploration and analysis of reaction mechanisms. *Journal of Computational Chemistry*, 40(25):2227–2233, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sen:2015:UGA

[SSSM15] Avijit Sen, Sangita Sen, Pradipta Kumar Samanta, and Debashis Mukherjee. Unitary group adapted state specific multireference perturbation theory: Formulation and pilot applications. *Journal of Computational Chemistry*, 36(9):670–688, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sugiura:2018:ROV

[SST+18] Yutaro Sugiura, Kento Suzuki, Toshiyuki Takayanagi, Yukiumi Kita, and Masanori Tachikawa. Reduction of OH vibrational frequencies in amino acids by positron attachment. *Journal of Computational Chemistry*, 39(25):2060–2066, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shen:2014:PTA

[SSWX14] Tonghao Shen, Neil Qiang Su, Anan Wu, and Xin Xu. Perturbative treatment of anharmonic vibrational effects on bond distances: an extended Langevin dynamics method. *Journal of Computational Chemistry*, 35(6):467–478, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2014:RCC

[SSX+14] Zhi Sun, Henry F. Schaefer III, Yaoming Xie, Yongdong Liu, and Rugang Zhong. The reactions of $Cr(CO)_6$, $Fe(CO)_5$, and $Ni(CO)_4$ with O_2 yield viable oxo-metal carbonyls. *Journal of Computational Chemistry*, 35(13):998–1009, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sapay:2011:CCF

[ST11] Nicolas Sapay and D. Peter Tieleman. Combination of the CHARMM27 force field with united-atom lipid force fields. *Journal of Computational Chemistry*, 32(7):1400–1410, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Singh:2013:REL

[ST13] Raman K. Singh and Takao Tsuneda. Reaction energetics on long-range corrected density functional theory: Diels–Alder reactions. *Journal of Computational Chemistry*, 34(5):379–386, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwalbe:2019:IAG

[STF+19] Sebastian Schwalbe, Kai Trepte, Lenz Fiedler, Alex I. Johnson, Jakob Kraus, Torsten Hahn, Juan E. Peralta, Koblar A. Jackson, and Jens Kortus. Interpretation and automatic generation of Fermi-orbital descriptors. *Journal of Computational Chemistry*, 40(32):2843–2857, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steffen:2010:TGU

[STH+10] Claudia Steffen, Klaus Thomas, Uwe Huniar, Arnim Hellweg, Oliver Rubner, and Alexander Schroer. TmoleX — a graphical user interface for TURBOMOLE. *Journal of Computational Chemistry*, 31(16):2967–2970, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stiebritz:2015:MPD

[Sti15] Martin T. Stiebritz. MetREx: a protein design approach for the exploration of sequence-reactivity relationships in metalloenzymes. *Journal of Computational Chemistry*, 36(8):553–563, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2015:CRS

[STM+15] Pin-Chih Su, Cheng-Chieh Tsai, Shahila Mehboob, Kirk E. Hevener, and Michael E. Johnson. Comparison of radii sets, entropy, QM methods, and sampling on MM–PBSA, MM–GBSA, and QM/MM–GBSA ligand binding energies of *F. tularensis* enoyl-ACP reductase (FabI). *Journal of Computational Chemistry*, 36(25):1859–1873, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sumiya:2017:FRC

[STM17] Yosuke Sumiya, Tetsuya Taketsugu, and Satoshi Maeda. Full rate constant matrix contraction method for obtaining branching ratio of unimolecular decomposition. *Journal of Computational Chemistry*, 38(2):101–109, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2010:TKS

[STS+10] Jingyu Sun, Yizhen Tang, Hao Sun, Xiujuan Jia, Xiumei Pan, and Rongshun Wang. Theoretical and kinetic study of the H + C_2H_5CN reaction. *Journal of Computational Chemistry*, 31(6):1126–1134, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sure:2015:SSR

[STS15] Rebecca Sure, Ralf Tonner, and Peter Schwerdtfeger. A systematic study of rare gas atoms encapsulated in small fullerenes using dispersion corrected density functional theory. *Journal of Computational Chemistry*, 36(2):88–96, January 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2010:CSP

[Su10] Ming-Der Su. A computational study of photochemical isomerization reactions of thiophenes. *Journal of Computational Chemistry*, 31(1):43–56, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2015:LEG

[Sun15] Qiming Sun. Libcint: an efficient general integral library for Gaussian basis functions. *Journal of Computational Chemistry*, 36(22):1664–1671, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sunda:2011:MDS

[SV11] Anurag Prakash Sunda and Arun Venkatnathan. Molecular dynamics simulations of triflic acid and triflate ion/water mixtures: a proton conducting electrolytic component in fuel cells. *Journal of Computational Chemistry*, 32(15):3319–3328, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sim:2015:HDH

[SV15] Adelene Y. L. Sim and Chandra Verma. How does a hydrocarbon staple affect peptide hydrophobicity? *Journal of Computational Chemistry*, 36(10):773–784, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Speldrich:2018:CUS

[SvLK18] Manfred Speldrich, Jan van Leusen, and Paul Kögerler. CONDON 3.0: An updated software package for magnetochemical analysis — all the way to polynuclear actinide complexes. *Journal of Computational Chemistry*, 39(25):2133–2145, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwerdtfeger:2013:SNU

[SWA13] Peter Schwerdtfeger, Lukas Wirz, and James Avery. Software news and updates: Program Fullerene: a software package for constructing and analyzing structures of regular fullerenes. *Journal of Computational Chemistry*, 34(17):1508–1526, June 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Strunk:2012:SNU

[SWB+12] T. Strunk, M. Wolf, M. Brieg, K. Klenin, A. Biewer, F. Tristram, M. Ernst, P. J. Kleine, N. Heilmann, I. Kondov, and W. Wenzel. Software news and updates: SIMONA 1.0: an efficient and versatile framework for stochastic simulations of molecular and nanoscale systems. *Journal of Computational Chemistry*, 33(32):2602–2613, December 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schnupf:2010:PDM

[SWM10] Udo Schnupf, J. L. Willett, and Frank A. Momany. 27 ps DFT molecular dynamics simulation of α-maltose: a reduced basis set study. *Journal of Computational Chemistry*, 31(11):2087–2097, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2010:HMP

[SWMW10] Weiyu Song, Jing Wang, Jian Meng, and Zhijian Wu. Half metallic properties of $LaSrVMoO_6$. *Journal of Computational Chemistry*, 31(9):1795–1798, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shi:2011:MEH

[SWPR11] Yue Shi, Chuanjie Wu, Jay W. Ponder, and Pengyu Ren. Multipole electrostatics in hydration free energy calculations. *Journal of Computational Chemistry*, 32(5):967–977, April 15,

2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2019:DNI

[SWW+19] He Su, Hui Wang, Hongyan Wang, Yunxiang Lu, and Zhengdan Zhu. Description of noncovalent interactions involving π-system with high precision: an assessment of RPA, MP2, and DFT-D methods. *Journal of Computational Chemistry*, 40(17):1643–1651, June 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shyu:2011:AES

[SY11] Conrad Shyu and F. Marty Ytreberg. Accurate estimation of solvation free energy using polynomial fitting techniques. *Journal of Computational Chemistry*, 32(1):134–141, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spassov:2016:PDC

[SY16a] Velin Z. Spassov and Lisa Yan. A pH-dependent computational approach to the effect of mutations on protein stability. *Journal of Computational Chemistry*, 37(29):2573–2587, November 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2016:TDT

[SY16b] Jiaye Su and Keda Yang. Temperature dependence of the transport of single-file water molecules through a hydrophobic channel. *Journal of Computational Chemistry*, 37(12): 1043–1047, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharabi:2011:OEF

[SYDS11] Oz Sharabi, Chen Yanover, Ayelet Dekel, and Julia M. Shifman. Optimizing energy functions for protein–protein interface design. *Journal of Computational Chemistry*, 32(1):23–32, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sindhikara:2012:PAP

[SYH12] Daniel J. Sindhikara, Norio Yoshida, and Fumio Hirata. Placevent: an algorithm for prediction of explicit solvent atom distribution — application to HIV-1 protease and F-ATP synthase. *Journal of Computational Chemistry*, 33(18): 1536–1543, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Solovyov:2012:MEU

[SYN+12] Ilia A. Solov'yov, Alexander V. Yakubovich, Pavel V. Nikolaev, Ilya Volkovets, and Andrey V. Solov'yov. MesoBioNano explorer — a universal program for multiscale computer simulations of complex molecular structure and dynamics. *Journal of Computational Chemistry*, 33(30):2412–2439, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2017:AVW

[SYZ+17] Lei Sun, Li Yang, Ya-Dong Zhang, Qi Shi, Rui-Feng Lu, and Wei-Qiao Deng. Accurate van der Waals force field for gas adsorption in porous materials. *Journal of Computational Chemistry*, 38(23):1991–1999, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sandhiya:2017:BHH

[SZ17] Lakshmanan Sandhiya and Hendrik Zipse. O–O bond homolysis in hydrogen peroxide. *Journal of Computational Chemistry*, 38(25):2186–2192, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2019:DRP

[SZB19] Xiufang Song, Fengying Zhang, and Yuxiang Bu. Dynamic relaying properties of a β-turn peptide in long-range electron transfer. *Journal of Computational Chemistry*, 40(9):988–996, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shim:2013:AXA

[SZBM13] Jihyun Shim, Xiao Zhu, Robert B. Best, and Alexander D. MacKerell Jr. (ala)$_4$ -X-(Ala)$_4$ as a model system for the optimization of the χ_1 and χ_2 amino acid side-chain dihedral empirical force field parameters. *Journal of Computational Chemistry*, 34(7):593–603, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Samsonov:2019:MLP

[SZdB19] Sergey A. Samsonov, Martin Zacharias, and Isaure Chauvot de Beauchene. Modeling large protein-glycosaminoglycan complexes using a fragment-based approach. *Journal of Computational Chemistry*, 40(14):1429–1439, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sheong:2019:RSN

[SZL19] FuKit Sheong, Jing-Xuan Zhang, and Zhenyang Lin. Revitalizing spin natural orbital analysis: Electronic structures of mixed-valence compounds, singlet biradicals, and antiferromagnetically coupled systems. *Journal of Computational Chemistry*, 40(10):1172–1184, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schupbach:2010:FTC

[SZTSM10] Thierry Schüpbach, Vincent Zoete, Brice Tsakam-Sotché, and Olivier Michielin. Fourier transform convolution integrals applied to generalized Born molecular volume. *Journal of Computational Chemistry*, 31(3):649–659, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2013:ADX

[SZX13a] Neil Qiang Su, Igor Ying Zhang, and Xin Xu. Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. *Journal of Computational Chemistry*, 34(20):1759–1774, July 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [SZX13b].

Su:2013:EAD

[SZX13b] Neil Qiang Su, Igor Ying Zhang, and Xin Xu. Erratum: Analytic derivatives for the XYG3 type of doubly hybrid density functionals: Theory, implementation, and assessment. *Journal of Computational Chemistry*, 34(27):2398–2399, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SZX13a].

Sun:2018:CPD

[SZZ+18] Chuancai Sun, Lijuan Zhu, Chao Zhang, Ce Song, Cuihong Wang, Meiling Zhang, Yaoming Xie, and Henry F. Schaefer

III. Conformers, properties, and docking mechanism of the anticancer drug docetaxel: DFT and molecular dynamics studies. *Journal of Computational Chemistry*, 39(15):889–900, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2016:TSE

[SZZS16] Haitao Sun, Shian Zhang, Cheng Zhong, and Zhenrong Sun. Theoretical study of excited states of DNA base dimers and tetramers using optimally tuned range-separated density functional theory. *Journal of Computational Chemistry*, 37(7): 684–693, March 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tachikawa:2017:EZP

[Tac17] Hiroto Tachikawa. Effects of zero point vibration on the reaction dynamics of water dimer cations following ionization. *Journal of Computational Chemistry*, 38(17):1503–1508, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tachibana:2019:NAQ

[Tac19] Akitomo Tachibana. New aspects of quantum electrodynamics on electronic structure and dynamics. *Journal of Computational Chemistry*, 40(2):316–327, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tomlinson:2016:NAS

[TAG16] David G. Tomlinson, Andrey Asadchev, and Mark S. Gordon. A new approach for second-order perturbation theory. *Journal of Computational Chemistry*, 37(14):1274–1282, May 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takeuchi:2010:GMG

[Tak10] Hiroshi Takeuchi. Global minimum geometries of acetylene clusters $(HCCH)_n$ with $n \leq 55$ obtained by a heuristic method combined with geometrical perturbations. *Journal of Computational Chemistry*, 31(8):1699–1706, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takeuchi:2011:TIO

[Tak11] Hiroshi Takeuchi. A theoretical investigation on optimal structures of ethane clusters $(C_2H_6)_n$ with $n \leq 25$ and their building-up principle. *Journal of Computational Chemistry*, 32(7):1345–1352, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takahashi:2014:DRF

[Tak14] Kazuaki Z. Takahashi. Design of a reaction field using a linear-combination-based isotropic periodic sum method. *Journal of Computational Chemistry*, 35(11):865–875, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takeuchi:2018:SGM

[Tak18] Hiroshi Takeuchi. Size-guided multi-seed heuristic method for geometry optimization of clusters: Application to benzene clusters. *Journal of Computational Chemistry*, 39(22):1738–1746, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tantardini:2019:WDH

[Tan19] Christian Tantardini. When does a hydrogen bond become a van der Waals interaction? a topological answer. *Journal of Computational Chemistry*, 40(8):937–943, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Turcani:2018:SPT

[TBJ18] Lukas Turcani, Enrico Berardo, and Kim E. Jelfs. `stk`: a Python toolkit for supramolecular assembly. *Journal of Computational Chemistry*, 39(23):1931–1942, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tan:2012:CSP

[TBSM12] Jeffrey S. Tan, Stephan X. M. Boerrigter, Raymond P. Scaringe, and Kenneth R. Morris. Core-shell potential-derived point charges. *Journal of Computational Chemistry*, 33(9):950–957, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tantardini:2016:SFP

[TCB16] Christian Tantardini, Davide Ceresoli, and Enrico Benassi. Source function and plane waves: Toward complete Bader analysis. *Journal of Computational Chemistry*, 37(23):2133–2139, September 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thomas:2013:PGF

[TCC+13] Dennis G. Thomas, Jaehun Chun, Zhan Chen, Guowei Wei, and Nathan A. Baker. Parameterization of a geometric flow implicit solvation model. *Journal of Computational Chemistry*, 34(8):687–695, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tobias:2018:DTK

[TCGNT18] Roland Tóbiás, Attila G. Császár, László Gyevi-Nagy, and Gyula Tasi. Definitive thermochemistry and kinetics of the interconversions among conformers of n-butane and n-pentane. *Journal of Computational Chemistry*, 39(8):424–437, March 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Torres:2014:TSR

[TCPPC14] Ana E. Torres, Guadalupe Castro, Ricardo Pablo-Pedro, and Fernando Colmenares. A two-step reaction scheme leading to singlet carbene species that can be detected under matrix conditions for the reaction of Zr(^{3} F) with either CH_3F or CH_3CN. *Journal of Computational Chemistry*, 35(11):883–890, April 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tu:2013:PFE

[TCX+13] Bin Tu, Minxin Chen, Yan Xie, Linbo Zhang, Bob Eisenberg, and Benzhuo Lu. A parallel finite element simulator for ion transport through three-dimensional ion channel systems. *Journal of Computational Chemistry*, 34(24):2065–2078, September 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tawari:2010:PME

[TD10] Nilesh R. Tawari and Mariam S. Degani. Pharmacophore mapping and electronic feature analysis for a series of nitroaromatic compounds with antitubercular activity. *Journal of Computational Chemistry*, 31(4):739–751, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tokmachev:2011:HBN

[TD11] A. M. Tokmachev and R. Dronskowski. Hydrogen-bond networks in finite ice nanotubes. *Journal of Computational Chemistry*, 32(1):99–105, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2010:DMA

[TDKT10] Athanassios C. Tsipis, Ioannis G. Depastas, Efstathios E. Karagiannis, and Constantinos A. Tsipis. Diagnosis of magnetoresponsive aromatic and antiaromatic zones in three-membered rings of d- and f-block elements. *Journal of Computational Chemistry*, 31(2):431–446, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taxak:2012:MIC

[TDP+12] Nikhil Taxak, Prashant V. Desai, Bhargav Patel, Michael Mohutsky, Valentine J. Klimkowski, Vijay Gombar, and Prasad V. Bharatam. Metabolic-intermediate complex formation with cytochrome P450: Theoretical studies in elucidating the reaction pathway for the generation of reactive nitroso intermediate. *Journal of Computational Chemistry*, 33 (21):1740–1747, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tupikina:2019:AFH

[TDT19] Elena Yu. Tupikina, Gleb S. Denisov, and Peter M. Tolstoy. Anticooperativity of $FH\cdots Cl^-$ hydrogen bonds in $[FH_n\ Cl]^-$ clusters ($n = 1 \ldots 6$). *Journal of Computational Chemistry*, 40(32):2858–2867, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tupikina:2018:OES

[TEDT18] Elena Yu. Tupikina, Alexandra A. Efimova, Gleb S. Denisov, and Peter M. Tolstoy. Outer electronic shell visualization by NMR chemical shift Laplacian of a helium probe. *Journal of Computational Chemistry*, 39(29):2459–2462, November 5,

2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thackston:2015:PLC

[TF15] Russell Thackston and Ryan C. Fortenberry. The performance of low-cost commercial cloud computing as an alternative in computational chemistry. *Journal of Computational Chemistry*, 36(12):926–933, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2010:ESN

[TFQ+10] Shu-Wei Tang, Jing-Dong Feng, Yong-Qing Qiu, Hao Sun, Feng-Di Wang, Ying-Fei Chang, and Rong-Shun Wang. Electronic structures and nonlinear optical properties of highly deformed halofullerenes C_{3v} $C_{60}F_{18}$ and D_{3d} $C_{60}Cl_{30}$. *Journal of Computational Chemistry*, 31(14):2650–2657, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2011:TSE

[TFQ+11] Shu-Wei Tang, Jing-Dong Feng, Yong-Qing Qiu, Hao Sun, Feng-Di Wang, Zhong-Min Su, Ying-Fei Chang, and Rong-Shun Wang. Thermochemical stabilities, electronic structures, and optical properties of $C_{56}X_{10}$ (X = H, F, and Cl) fullerene compounds. *Journal of Computational Chemistry*, 32(4):658–667, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takeda:2019:MDS

[TFYO19] Kosuke Takeda, Kazushi Fujimoto, Noriyuki Yoshii, and Susumu Okazaki. Molecular dynamics study of solubilization of cyclohexane, benzene, and phenol into mixed micelles composed of sodium dodecyl sulfate and octaethylene glycol monododecyl ether. *Journal of Computational Chemistry*, 40(31):2722–2729, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tonigold:2012:DIW

[TG12a] Katrin Tonigold and Axel Groß. Dispersive interactions in water bilayers at metallic surfaces: a comparison of the PBE and RPBE functional including semiempirical dispersion corrections. *Journal of Computational Chemistry*, 33(6):695–701, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2012:PES

[TG12b] Athanassios C. Tsipis and Dimitrios N. Gkarmpounis. Probing the electronic structure, chemical bonding, and excitation spectra of $[CuE]^{+/0/-}$ (E = 14 group element) diatomics employing DFT and ab initio methods. *Journal of Computational Chemistry*, 33(29):2318–2331, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Teodoro:2013:ARA

[TH13] Tiago Quevedo Teodoro and Roberto Luiz Andrade Haiduke. Accurate relativistic adapted Gaussian basis sets for francium through ununoctium without variational prolapse and to be used with both uniform sphere and Gaussian nucleus models. *Journal of Computational Chemistry*, 34(27):2372–2379, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takenaka:2019:FPC

[THI+19] Masato Takenaka, Yoshikazu Hashimoto, Takeshi Iwasa, Tetsuya Taketsugu, Gediminas Seniutinas, Armandas Balcytis, Saulius Juodkazis, and Yoshiaki Nishijima. First Principles Calculations Toward Understanding SERS of 2,2'-Bipyridyl Adsorbed on Au, Ag, and Au-Ag Nanoalloy. *Journal of Computational Chemistry*, 40(8):925–932, March 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tam:2015:BST

[THP+15] Nguyen Minh Tam, Tran Dieu Hang, Hung Tan Pham, Huyen Thi Nguyen, My Phuong Pham-Ho, Pablo A. Denis, and Minh Tho Nguyen. Bonding and singlet–triplet gap of silicon trimer: Effects of protonation and attachment of alkali metal cations. *Journal of Computational Chemistry*, 36(11): 805–815, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tian:2012:MNO

[Tia12] Wei Quan Tian. Modeling nonlinear optics of nanosystems with sum-over-states model. *Journal of Computational Chem-*

istry, 33(4):466–470, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tyka:2012:ESP

[TJB12] Michael D. Tyka, Kenneth Jung, and David Baker. Efficient sampling of protein conformational space using fast loop building and batch minimization on highly parallel computers. *Journal of Computational Chemistry*, 33(31):2483–2491, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thapa:2019:EMI

[TJR19] Mahendra Thapa, Eric Johnson, and Mark Rance. Effect of monovalent ion binding on molecular dynamics of the S100-family calcium-binding protein calbindin D_{9k}. *Journal of Computational Chemistry*, 40(22):1936–1945, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tuer:2011:TDV

[TKC+11] Adam Tuer, Serguei Krouglov, Richard Cisek, Danielle Tokarz, and Virginijus Barzda. Three-dimensional visualization of the first hyperpolarizability tensor. *Journal of Computational Chemistry*, 32(6):1128–1134, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trung:2019:RSC

[TKCN19] Nguyen Tien Trung, Pham Ngoc Khanh, Alfredo J. Palace Carvalho, and Minh Tho Nguyen. Remarkable shifts of C_{sp2}-H and O-H stretching frequencies and stability of complexes of formic acid with formaldehydes and thioformaldehydes. *Journal of Computational Chemistry*, 40(13):1387–1400, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanaka:2013:ORM

[TKN13] Masato Tanaka, Michio Katouda, and Shigeru Nagase. Optimization of RI-MP2 Auxiliary Basis Functions for 6-31G** and 6-311G** basis sets for first-, second-, and third-row elements. *Journal of Computational Chemistry*, 34(29):2568–2575, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takenaka:2010:OSS

[TKNN10] Norio Takenaka, Yoshiyuki Koyano, Yukinori Nakagawa, and Masataka Nagaoka. An optimum strategy for solution chemistry using semiempirical molecular orbital method: Importance of description of charge distribution. *Journal of Computational Chemistry*, 31(6):1287–1296, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Terakawa:2011:EIV

[TKT11] Tsuyoshi Terakawa, Tomoshi Kameda, and Shoji Takada. On easy implementation of a variant of the replica exchange with solute tempering in GROMACS. *Journal of Computational Chemistry*, 32(7):1228–1234, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Talipov:2013:CDN

[TKXT13] Marat R. Talipov, Dmitry G. Khomyakov, Ming Xian, and Qadir K. Timerghazin. Computational design of S-nitrosothiol “click” reactions. *Journal of Computational Chemistry*, 34(18):1527–1530, July 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanaka:2017:SPS

[TKYN17] Yuichi Tanaka, Yukio Kawashima, Norio Yoshida, and Haruyuki Nakano. Solvatochromism and preferential solvation of Brooker’s merocyanine in water–methanol mixtures. *Journal of Computational Chemistry*, 38(28):2411–2419, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tusar:2016:HBH

[TL16] Simona Tušar and Antonija Lesar. Hydrogen bonding in the hydroxysulfinyl radical-formic acid-water system: a theoretical study. *Journal of Computational Chemistry*, 37(17):1611–1625, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tognetti:2010:HCC

[TLA10] Vincent Tognetti, Pascal Le Floch, and Carlo Adamo. How the choice of a computational model could rule the chemical interpretation: the Ni(II) catalyzed ethylene dimerization as a case study. *Journal of Computational Chemistry*, 31(5):1053–1062, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tabookht:2012:RBM

[TLdG+12] Zahra Tabookht, Xavier López, Coen de Graaf, Nathalie Guihéry, Nicolas Suaud, and Nadia Benamor. Rationalization of the behavior of M_2 $(CH_3CS_2)_4I$ (M = Ni, Pt) chains at room temperature from periodic density functional theory and ab initio cluster calculations. *Journal of Computational Chemistry*, 33(21):1748–1761, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2012:CFF

[TLY+12] Hao Tang, Zhuo Li, Yu-Hong Yang, Ying Zhao, Su-Qin Wan, Hui-Ling Liu, and Xu-Ri Huang. Comparison of the FeO^{2+} and FeS^{2+} complexes in the cyanide and isocyanide ligand environment for methane hydroxylation. *Journal of Computational Chemistry*, 33(16):1448–1457, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tahat:2016:MEV

[TM16] Amani Tahat and Jordi Martí. Multistate empirical valence bond study of temperature and confinement effects on proton transfer in water inside hydrophobic nanochannels. *Journal of Computational Chemistry*, 37(20):1935–1946, July 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takahashi:2018:REA

[TM18] Keisuke Takahashi and Itsuki Miyazato. Rapid estimation of activation energy in heterogeneous catalytic reactions via machine learning. *Journal of Computational Chemistry*, 39(28):2405–2408, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tognetti:2015:QEN

[TMJ15] Vincent Tognetti, Christophe Morell, and Laurent Joubert. Quantifying electro/nucleophilicity by partitioning the dual descriptor. *Journal of Computational Chemistry*, 36(9):649–659, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takano:2010:ESH

[TN10] Yu Takano and Haruki Nakamura. Electronic structures of heme *a* of cytochrome *c* oxidase in the redox states — charge density migration to the propionate groups of heme *a*. *Journal of Computational Chemistry*, 31(5):954–962, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tai:2012:EST

[TN12] Truong Ba Tai and Minh Tho Nguyen. Electronic structure and thermochemical properties of silicon-doped lithium clusters $Li_nSi^{0/+}$, $n = 1$–8: New insights on their stability. *Journal of Computational Chemistry*, 33(7):800–809, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takayanagi:2018:ARP

[TN18] Toshiyuki Takayanagi and Taiki Nakatomi. Automated reaction path searches for spin-forbidden reactions. *Journal of Computational Chemistry*, 39(19):1319–1326, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Truchon:2010:UEP

[TNG+10] Jean-François Truchon, Anthony Nicholls, J. Andrew Grant, Radu I. Iftimie, Benoît Roux, and Christopher I. Bayly. Using electronic polarization from the internal continuum (EPIC) for intermolecular interactions. *Journal of Computational Chemistry*, 31(4):811–824, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takagi:2019:EPN

[TNI+19a] Nozomi Takagi, Masayuki Nakagaki, Kazuya Ishimura, Ryoichi Fukuda, Masahiro Ehara, and Shigeyoshi Sakaki. Electronic processes in NO dimerization on Ag and Cu clusters: DFT and MRMP2 studies. *Journal of Computational Chemistry*, 40(1):181–190, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tran:2019:RPC

[TNI19b] Kelly N. Tran, Shuqiang Niu, and Toshiko Ichiye. Reduction potential calculations of the Fe-S clusters in Thermus thermophilus respiratory complex I. *Journal of Computational Chemistry*, 40(12):1248–1256, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tonddast-Navaei:2017:ICP

[TNSS17] Sam Tonddast-Navaei, Bharath Srinivasan, and Jeffrey Skolnick. On the importance of composite protein multiple ligand interactions in protein pockets. *Journal of Computational Chemistry*, 38(15):1252–1259, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takayanagi:2018:IPD

[TNY18] Toshiyuki Takayanagi, Taiki Nakatomi, and Yoshiteru Yonetani. On the ion-pair dissociation mechanisms in the small NaCl$\cdot$ $(H_2O)_6$ cluster: a perspective from reaction path search calculations. *Journal of Computational Chemistry*, 39(23): 1835–1842, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Takano:2016:SNU

[TNYN16] Yu Takano, Kazuto Nakata, Yasushige Yonezawa, and Haruki Nakamura. Software news and updates: Development of massive multilevel molecular dynamics simulation program, PLATYpus (PLATform for dYnamic protein unified simulation), for the elucidation of protein functions. *Journal of Computational Chemistry*, 37(12):1125–1132, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trott:2010:AVI

[TO10] Oleg Trott and Arthur J. Olson. AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *Journal of Computational Chemistry*, 31(2):455–461, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taju:2019:DDL

[TO19] Semmy Wellem Taju and Yu-Yen Ou. DeepIon: Deep learning approach for classifying ion transporters and ion channels from membrane proteins. *Journal of Computational Chemistry*, 40(15):1521–1529, June 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tan:2010:TIE

[TPL+10] Bisheng Tan, Rufang Peng, Hongbo Li, Bo Jin, Shijin Chu, and Xinping Long. Theoretical investigation of an energetic fullerene derivative. *Journal of Computational Chemistry*, 31 (12):2233–2237, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Turcheniuk:2012:PVI

[TR12] K. V. Turcheniuk and A. B. Rozhenko. (σ^3, λ^5)-phosphoranes versus (σ^3, λ^3)-thiaphosphiranes: Quantum chemical investigation of products of phosphaalkene sulfurization. *Journal of Computational Chemistry*, 33(10):1023–1028, April 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Traore:2016:FSA

[TRA+16] Seydou Traoré, Kyle E. Roberts, David Allouche, Bruce R. Donald, Isabelle André, Thomas Schiex, and Sophie Barbe. Fast search algorithms for computational protein design. *Journal of Computational Chemistry*, 37(12):1048–1058, May 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trumm:2018:IIM

[Tru18] Michael Trumm. On the isotropy of induced multipole moments in heavy ion complexes. *Journal of Computational Chemistry*, 39(7):373–379, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tao:2010:TAO

[TS10a] Peng Tao and H. Bernhard Schlegel. A toolkit to assist ONIOM calculations. *Journal of Computational Chemistry*, 31(12):2363–2369, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsalavoutis:2010:DFI

[TS10b] John T. Tsalavoutis and Michael P. Sigalas. Density functional investigation and bonding analysis of pentacoordinated iron complexes with mixed cyano and carbonyl ligands. *Journal of Computational Chemistry*, 31(10):1969–1978, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2011:SEM

[TS11] Athanassios C. Tsipis and Alexandros V. Stalikas. Structural, electronic, and magnetoresponsive properties of triangular lanthanide clusters and their free-standing nitrides. *Journal of Computational Chemistry*, 32(4):620–638, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuneda:2014:RIB

[TS14] Takao Tsuneda and Raman K. Singh. Reactivity index based on orbital energies. *Journal of Computational Chemistry*, 35 (14):1093–1100, May 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thenraj:2015:CER

[TS15a] Murugesan Thenraj and Ashoka G. Samuelson. Contrasting electronic requirements for C H binding and C H activation in d^6 half-sandwich complexes of rhenium and tungsten. *Journal of Computational Chemistry*, 36(24):1818–1830, September 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2015:EBO

[TS15b] Athanassios C. Tsipis and Alexandros V. Stalikas. Electronic, bonding, and optical properties of 1 d $[CuCN]_n$ (n = 1–10) chains, 24 d $[Cu\ CN]_n$ ($n = 2 - 10$) nanorings, and 3 d $[Cu_n (CN)_n]_m$ ($n = 4$, $m = 2, 3$; $n = 10$, $m = 2$) tubes studied by DFT /TD–DFT methods. *Journal of Computational Chemistry*, 36(17):1334–1347, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thellamurege:2013:SNU

[TSC+13] Nandun M. Thellamurege, Dejun Si, Fengchao Cui, Hongbo Zhu, Rui Lai, and Hui Li. Software news and updates: QuanPol: a full spectrum and seamless QM/MM program. *Journal of Computational Chemistry*, 34(32):2816–2833, December 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trepte:2019:AAG

[TSH+19] Kai Trepte, Sebastian Schwalbe, Torsten Hahn, Jens Kortus, Der-You Kao, Yoh Yamamoto, Tunna Baruah, Rajendra R.

Zope, Kushantha P. K. Withanage, Juan E. Peralta, and Koblar A. Jackson. Analytic atomic gradients in the Fermi–Löwdin orbital self-interaction correction. *Journal of Computational Chemistry*, 40(6):820–825, March 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2014:DAS

[Tsi14] Athanassios C. Tsipis. DFT assessment of the spectroscopic constants and absorption spectra of neutral and charged diatomic species of group 11 and 14 elements. *Journal of Computational Chemistry*, 35(24):1762–1777, September 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2017:EPR

[Tsi17] Athanassios C. Tsipis. Exploring possible reaction pathways for the o-atom transfer reactions to unsaturated substrates catalyzed by a [Ni-NO_2] [Ni-NO] redox couple using DFT methods. *Journal of Computational Chemistry*, 38(20):1780–1788, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsirelson:2018:EDQ

[Tsi18] Vladimir Tsirelson. Early days of quantum crystallography: a personal account. *Journal of Computational Chemistry*, 39 (17):1029–1037, June 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsipis:2019:TPT

[Tsi19] Athanassios C. Tsipis. Trans-philicity (trans-influence/trans-effect) ladders for square planar platinum(II) complexes constructed by ^{35}Cl NMR probe. *Journal of Computational Chemistry*, 40(29):2550–2562, November 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2010:MKI

[TSJ+10] Yizhen Tang, Jingyu Sun, Xiujuan Jia, Hao Sun, Xiumei Pan, and Rongshun Wang. Mechanistic and kinetic investigations of N_2H_4 + OH reaction. *Journal of Computational Chemistry*, 31(7):1520–1527, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuneda:2016:RBO

[TSN16] Takao Tsuneda, Raman K. Singh, and Ayako Nakata. Relationship between orbital energy gaps and excitation energies for long-chain systems. *Journal of Computational Chemistry*, 37(16):1451–1462, June 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuneda:2017:LLE

[TSN17] Takao Tsuneda, Raman K. Singh, and Ayako Nakata. On low-lying excited states of extended nanographenes. *Journal of Computational Chemistry*, 38(23):2020–2029, September 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Torrent-Sucarrat:2017:RDM

[TSNC+17] Miquel Torrent-Sucarrat, Sara Navarro, Fernando P. Cossío, Josep M. Anglada, and Josep M. Luis. Relevance of the DFT method to study expanded porphyrins with different topologies. *Journal of Computational Chemistry*, 38(32):2819–2828, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Torres:2016:SAA

[TSR+16] Ana M. Torres, Steve Scheiner, Ajit K. Roy, Andrés M. Garay-Tapia, John Bustamante, and Tapas Kar. Segmentation and additive approach: a reliable technique to study noncovalent interactions of large molecules at the surface of single-wall carbon nanotubes. *Journal of Computational Chemistry*, 37 (21):1953–1961, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuneda:2019:TIG

[Tsu19] Takao Tsuneda. Theoretical investigations on geometrical and electronic structures of silver clusters. *Journal of Computational Chemistry*, 40(1):206–211, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [NSN19].

Tang:2012:TMG

[TSZQ12] Lingli Tang, Linwei Sai, Jijun Zhao, and Ruifeng Qiu. A topological method for global optimization of clusters: Application to $(TiO_2)_n$ ($n = 1$–6). *Journal of Computational Chemistry*, 33(2):163–169, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tran:2018:SSE

[TT18] Van Tan Tran and Quoc Tri Tran. Spin state energetics of $VGe_n^{-/0}$ ($n = 5$–7) clusters and new assignments of the anion photoelectron spectra. *Journal of Computational Chemistry*, 39(25):2103–2109, September 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Toropov:2010:SBO

[TTB+10] Andrey A. Toropov, Alla P. Toropova, Emilio Benfenati, Danuta Leszczynska, and Jerzy Leszczynski. SMILES-based optimal descriptors: QSAR analysis of fullerene-based HIV-1 PR inhibitors by means of balance of correlations. *Journal of Computational Chemistry*, 31(2):381–392, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Toropova:2011:CQS

[TTB+11] A. P. Toropova, A. A. Toropov, E. Benfenati, G. Gini, D. Leszczynska, and J. Leszczynski. CORAL: Quantitative structure–activity relationship models for estimating toxicity of organic compounds in rats. *Journal of Computational Chemistry*, 32(12):2727–2733, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Thompson:2018:PPC

[TTC+18] Helen Nathalia Thompson, Claudia Elizabeth Thompson, Rafael Andrade Caceres, Laurent Emmanuel Dardenne, Paulo Augusto Netz, and Hubert Stassen. Prion protein conversion triggered by acidic condition: a molecular dynamics study through different force fields. *Journal of Computational Chemistry*, 39(24):2000–2011, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Toropova:2012:SNU

[TTL+12] A. P. Toropova, A. A. Toropov, A. Lombardo, A. Roncaglioni, E. Benfenati, and G. Gini. Software news and updates: Coral: QSAR models for acute toxicity in fathead minnow (*Pimephales promelas*). *Journal of Computational Chemistry*, 33(12):1218–1223, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuchimochi:2019:ESS

[TTn19] Takashi Tsuchimochi and Seiichiro L. Ten-no. Extending spin-symmetry projected coupled-cluster to large model spaces using an iterative null-space projection technique. *Journal of Computational Chemistry*, 40(1):265–278, January 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Toropov:2012:SNU

[TTR+12] A. A. Toropov, A. P. Toropova, B. F. Rasulev, E. Benfenati, G. Gini, D. Leszczynska, and J. Leszczynski. Software news and updates: Coral: QSPR modeling of rate constants of reactions between organic aromatic pollutants and hydroxyl radical. *Journal of Computational Chemistry*, 33(23):1902–1906, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Torii:2010:PHA

[TY10] Hajime Torii and Masaki Yoshida. Properties of halogen atoms for representing intermolecular electrostatic interactions related to halogen bonding and their substituent effects. *Journal of Computational Chemistry*, 31(1):107–116, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanaka:2015:TDR

[TYN15] Yuichi Tanaka, Norio Yoshida, and Haruyuki Nakano. Three-dimensional reference interaction site model self-consistent field analysis of solvent and substituent effects on the absorption spectra of Brooker's merocyanine. *Journal of Computational Chemistry*, 36(22):1655–1663, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taherzadeh:2018:PLM

[TYX+18] Ghazaleh Taherzadeh, Yuedong Yang, Haodong Xu, Yu Xue, Alan Wee-Chung Liew, and Yaoqi Zhou. Predicting lysine-malonylation sites of proteins using sequence and predicted structural features. *Journal of Computational Chemistry*, 39 (22):1757–1763, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taherzadeh:2016:SBP

[TYZ+16] Ghazaleh Taherzadeh, Yuedong Yang, Tuo Zhang, Alan Wee-Chung Liew, and Yaoqi Zhou. Sequence-based prediction of protein–peptide binding sites using support vector machine. *Journal of Computational Chemistry*, 37(13):1223–1229, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tunega:2011:UBM

[TZ11] Daniel Tunega and Ali Zaoui. Understanding of bonding and mechanical characteristics of cementitious mineral tobermorite from first principles. *Journal of Computational Chemistry*, 32(2):306–314, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2012:DDB

[TZ12] Shanshan Tang and Jingping Zhang. Design of donors with broad absorption regions and suitable frontier molecular orbitals to match typical acceptors via substitution on oligo(thienylenevinylene) toward solar cells. *Journal of Computational Chemistry*, 33(15):1353–1363, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tao:2018:CVS

[TZCK18] Yunwen Tao, Wenli Zou, Dieter Cremer, and Elfi Kraka. Correlating the vibrational spectra of structurally related molecules: a spectroscopic measure of similarity. *Journal of Computational Chemistry*, 39(6):293–306, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Urquiza-Carvalho:2016:ASE

[UCFR16] Gabriel Aires Urquiza-Carvalho, Wallace Duarte Fragoso, and Gerd Bruno Rocha. Assessment of semiempirical enthalpy of formation in solution as an effective energy function to discriminate native-like structures in protein decoy sets. *Journal of Computational Chemistry*, 37(21):1962–1972, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Urquiza-Carvalho:2018:EAE

[UCRL18] Gabriel A. Urquiza-Carvalho, Gerd B. Rocha, and Rafael López. Efficient algorithm for expanding theoretical electron densities in Canterakis–Zernike functions. *Journal of Computational Chemistry*, 39(24):2022–2032, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Uppsten:2012:QCC

[UD12] Malin Uppsten and Bo Durbeej. Quantum chemical comparison of vertical, adiabatic, and 0–0 excitation energies: The PYP and GFP chromophores. *Journal of Computational Chemistry*, 33(23):1892–1901, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Unsleber:2018:SSQ

[UDK+18] Jan P. Unsleber, Thomas Dresselhaus, Kevin Klahr, David Schnieders, Michael Böckers, Dennis Barton, and Johannes Neugebauer. Serenity: a subsystem quantum chemistry program. *Journal of Computational Chemistry*, 39(13):788–798, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Utecht:2018:DIL

[UGK18] Manuel Utecht, Tina Gaebel, and Tillmann Klamroth. Desorption induced by low energy charge carriers on Si(111)-7×7: First principles molecular dynamics for benzene derivates. *Journal of Computational Chemistry*, 39(30):2517–2525, November 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Unni:2011:WSS

[UHH+11] Samir Unni, Yong Huang, Robert M. Hanson, Malcolm Tobias, Sriram Krishnan, Wilfred W. Li, Jens E. Nielsen, and Nathan A. Baker. Web servers and services for electrostatics calculations with APBS and PDB2PQR. *Journal of Computational Chemistry*, 32(7):1488–1491, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Umeda:2010:PFM

[UIW+10] Hiroaki Umeda, Yuichi Inadomi, Toshio Watanabe, Toru Yagi, Takayoshi Ishimoto, Tsutomu Ikegami, Hiroto Tadano, Tetsuya Sakurai, and Umpei Nagashima. Parallel Fock matrix construction with distributed shared memory model for the FMO–MO method. *Journal of Computational Chemistry*, 31(13):2381–2388, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Uhe:2011:AAC

[UKS11] Andreas Uhe, Sebastian Kozuch, and Sason Shaik. Automatic analysis of computed catalytic cycles. *Journal of Computational Chemistry*, 32(5):978–985, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lao:2011:CSU

[uLhY11] Ka un Lao and Chin hui Yu. A computational study of unique properties of pillar[n] quinones: Self-assembly to tubular structures and potential applications as electron acceptors and anion recognizers. *Journal of Computational Chemistry*, 32(12):2716–2726, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Uejima:2013:GOF

[UM13] Yutaka Uejima and Ryo Maezono. GPGPU for orbital function evaluation with a new updating scheme. *Journal of Computational Chemistry*, 34(2):83–94, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ueno-Noto:2016:WMI

[UNT16] Kaori Ueno-Noto and Keiko Takano. Water molecules inside protein structure affect binding of monosaccharides with HIV-1 antibody 2G12. *Journal of Computational Chemistry*, 37 (26):2341–2348, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Udagawa:2011:IMD

[US11] Taro Udagawa and Shogo Sakai. Ab initio molecular dynamics of protonated water clusters by integrated multicenter molecular-orbital method. *Journal of Computational Chemistry*, 32(13):2902–2908, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Udagawa:2014:WND

[UT14] Taro Udagawa and Masanori Tachikawa. Why is N···Be distance of $NH_3H^+\cdots DBeH$ shorter than that of $NH_3D^+\cdots HBeH$? Paradoxical geometrical isotope effects for partially isotope-substituted dihydrogen-bonded isotopomers. *Journal of Computational Chemistry*, 35(4):271–274, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Udagawa:2015:HDI

[UT15] Taro Udagawa and Masanori Tachikawa. H/D isotope effect on charge-inverted hydrogen-bonded systems: Systematic classification of three different types in $H_3\ XH\cdots YH_3$ (X = C, Si, or Ge, and Y = B, Al, or Ga) with multicomponent calculation. *Journal of Computational Chemistry*, 36 (22):1647–1654, August 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Uejima:2011:AQM

[UTM11] Yutaka Uejima, Tomoharu Terashima, and Ryo Maezono. Acceleration of a QM/MM-QMC simulation using GPU. *Journal of Computational Chemistry*, 32(10):2264–2272, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ullmann:2012:SNU

[UU12] R. Thomas Ullmann and G. Matthias Ullmann. Software news and updates: GMCT: a Monte Carlo simulation package for macromolecular receptors. *Journal of Computational Chemistry*, 33(8):887–900, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ungerer:2019:DFT

[UvSvdWK19] Maria Johanna Ungerer, Cornelia Gertina Catharina Elizabeth van Sittert, Derik Johannes van der Westhuizen, and Henning Manfred Krieg. Density functional theory study with and without COSMO of $H_2\ SO_4$ reactions in an aqueous environment for metal extraction. *Journal of Computational Chemistry*, 40(3):591–606, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venkatraman:2014:QSP

[VÅA14] Vishwesh Venkatraman, Per-Olof Åstrand, and Bjørn Kåre Alsberg. Quantitative structure–property relationship modeling of Grätzel solar cell dyes. *Journal of Computational Chemistry*, 35(3):214–226, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vonAppen:2014:IMS

[vADC+14] Jörg von Appen, Richard Dronskowski, Aurab Chakrabarty, Tilmann Hickel, Robert Spatschek, and Jörg Neugebauer. Impact of Mn on the solution enthalpy of hydrogen in austenitic Fe–Mn alloys: a first-principles study. *Journal of Computational Chemistry*, 35(31):2239–2244, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vila:2014:ACS

[VAMS14] Jorge A. Vila, Yelena A. Arnautova, Osvaldo A. Martin, and Harold A. Scheraga. Are accurate computations of the ^{13}C' shielding feasible at the DFT level of theory? *Journal of Computational Chemistry*, 35(4):309–312, February 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vega:2012:SNU

[VAR12] David Vega, Yosslen Aray, and Jesús Rodríguez. Software news and updates: C library for topological study of the electronic charge density. *Journal of Computational Chemistry*, 33(31):2526–2531, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanderWeeen:2011:DPS

[VBD11] Pieter Van der Weeën, Jan M. Baetens, and Bernard De Baets. Design and parameterization of a stochastic cellular automaton describing a chemical reaction. *Journal of Computational Chemistry*, 32(9):1952–1961, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Villalba:2011:CEM

[VBDS+11] J. M. Villalba, A. J. Barbero, R. Diaz-Sierra, E. Arribas, M. J. Garcia-Meseguer, F. Garcia-Sevilla, M. Garcia-Moreno, J. A. Vidal De Labra, and R. Varon. Computerized evaluation of mean residence times in multicompartmental linear system and pharmacokinetics. *Journal of Computational Chemistry*, 32(5):915–931, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viciano:2013:NIE

[VBMA13] Ignacio Viciano, Slawomir Berski, Sergio Martí, and Juan Andrés. New insight into the electronic structure of iron(IV)-oxo porphyrin compound I. A quantum chemical topological analysis. *Journal of Computational Chemistry*, 34(9):780–789, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanpoucke:2013:EHB

[VBV13a] Danny E. P. Vanpoucke, Patrick Bultinck, and Isabel Van Driessche. Extending Hirshfeld-I to bulk and periodic materials. *Journal of Computational Chemistry*, 34(5):405–417, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [Man13] and reply [VVB13].

Vysotskiy:2013:SNU

[VBV13b] Victor P. Vysotskiy, Jonas Boström, and Valera Veryazov. Software news and updates: a new module for constrained multi-fragment geometry optimization in internal coordinates implemented in the MOLCAS package. *Journal of Computational Chemistry*, 34(30):2657–2665, November 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vikramaditya:2018:INE

[VCL18] Talapunur Vikramaditya, Jeng-Da Chai, and Shiang-Tai Lin. Impact of non-empirically tuning the range-separation parameter of long-range corrected hybrid functionals on ionization potentials, electron affinities, and fundamental gaps. *Journal of Computational Chemistry*, 39(28):2378–2384, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viciano:2015:QMM

[VCM15] Ignacio Viciano, Raquel Castillo, and Sergio Martí. QM/MM modeling of the hydroxylation of the androstenedione substrate catalyzed by cytochrome P450 aromatase

(CYP19A1). *Journal of Computational Chemistry*, 36(23): 1736–1747, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vancoillie:2013:PMP

[VDL+13] Steven Vancoillie, Mickaël G. Delcey, Roland Lindh, Victor Vysotskiy, Per-Åke Malmqvist, and Valera Veryazov. Parallelization of a multiconfigurational perturbation theory. *Journal of Computational Chemistry*, 34(22):1937–1948, August 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vogt:2014:WIS

[VDVR14] Natalja Vogt, Jean Demaison, Jürgen Vogt, and Heinz Dieter Rudolph. Why it is sometimes difficult to determine the accurate position of a hydrogen atom by the semiexperimental method: Structure of molecules containing the OH or the CH_3 group. *Journal of Computational Chemistry*, 35(32): 2333–2342, December 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vener:2012:IHB

[VECT12] M. V. Vener, A. N. Egorova, A. V. Churakov, and V. G. Tsirelson. Intermolecular hydrogen bond energies in crystals evaluated using electron density properties: DFT computations with periodic boundary conditions. *Journal of Computational Chemistry*, 33(29):2303–2309, November 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VonAppen:2010:DFS

[VED10] Jörg Von Appen, Bernhard Eck, and Richard Dronskowski. A density-functional study of the phase diagram of cementite-type $(Fe,Mn)_3C$ at absolute zero temperature. *Journal of Computational Chemistry*, 31(14):2620–2627, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vela:2016:ZOH

[VFRAR16] Sergi Vela, Maria Fumanal, Jordi Ribas-Ariño, and Vincent Robert. On the zeroth-order Hamiltonian for CASPT2 calculations of spin crossover compounds. *Journal of Compu-*

tational Chemistry, 37(10):947–953, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vogt-Geisse:2016:CPR

[VGTL16] Stefan Vogt-Geisse and Alejandro Toro-Labbé. Chemical potential and reaction electronic flux in symmetry controlled reactions. *Journal of Computational Chemistry*, 37(19):1794–1800, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanfleteren:2011:FDM

[VGV+11] Diederik Vanfleteren, Dieter Ghillemijn, Dimitri Van Neck, Patrick Bultinck, Michel Waroquier, and Paul W. Ayers. Fast density matrix-based partitioning of the energy over the atoms in a molecule consistent with the hirshfeld-I partitioning of the electron density. *Journal of Computational Chemistry*, 32 (16):3485–3496, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanommeslaeghe:2010:CGF

[VHA+10] K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov, and A. D. Mackerell Jr. CHARMM general force field: a force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields. *Journal of Computational Chemistry*, 31(4):671–690, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vaucher:2016:RTF

[VHR16] Alain C. Vaucher, Moritz P. Haag, and Markus Reiher. Real-time feedback from iterative electronic structure calculations. *Journal of Computational Chemistry*, 37(9):805–812, April 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vujovic:2019:EAD

[VHS+19] Milena Vujović, Mioy Huynh, Sebastian Steiner, Pablo Garcia-Fernandez, Marcus Elstner, Qiang Cui, and Maja Gruden. Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin-polarized DFTB3 model. *Journal of Computa-*

tional Chemistry, 40(2):400–413, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vines:2017:ESS

[VI17] Francesc Viñes and Francesc Illas. Electronic structure of stoichiometric and reduced ZnO from periodic relativistic all electron hybrid density functional calculations using numeric atom-centered orbitals. *Journal of Computational Chemistry*, 38(8):523–529, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vikas:2011:MIS

[Vik11] Vikas. He molecular ion in a strong time-dependent magnetic field: a current-density functional study. *Journal of Computational Chemistry*, 32(11):2404–2413, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vach:2015:DIS

[VIT+15] Holger Vach, Lena V. Ivanova, Qadir K. Timerghazin, Fatme Jardali, and Ha-Linh Thi Le. A deeper insight into strain for the sila-bi[6]prismane ($Si_{18}H_{12}$) cluster with its endohedrally trapped silicon atom, $Si_{19}H_{12}$. *Journal of Computational Chemistry*, 36(28):2089–2094, October 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vardi-Kilshtain:2012:PIC

[VKAM12] Alexandra Vardi-Kilshtain, Asaf Azuri, and Dan Thomas Major. Path-integral calculations of heavy atom kinetic isotope effects in condensed phase reactions using higher-order Trotter factorizations. *Journal of Computational Chemistry*, 33 (4):435–441, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vilar:2010:LSB

[VKC10] Santiago Vilar, Joel Karpiak, and Stefano Costanzi. Ligand and structure-based models for the prediction of ligand-receptor affinities and virtual screenings: Development and application to the β_2-adrenergic receptor. *Journal of Computational Chemistry*, 31(4):707–720, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vasilevskaya:2015:MPM

[VKNT15] Tatiana Vasilevskaya, Maria G. Khrenova, Alexander V. Nemukhin, and Walter Thiel. Mechanism of proteolysis in matrix metalloproteinase-2 revealed by QM/MM modeling. *Journal of Computational Chemistry*, 36(21):1621–1630, August 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vasilevskaya:2016:MAQ

[VKNT16] Tatiana Vasilevskaya, Maria G. Khrenova, Alexander V. Nemukhin, and Walter Thiel. Methodological aspects of QM/MM calculations: a case study on matrix metalloproteinase-2. *Journal of Computational Chemistry*, 37(19):1801–1809, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vilseck:2015:ABG

[VKTRJ15] Jonah Z. Vilseck, Jakub Kostal, Julian Tirado-Rives, and William L. Jorgensen. Application of a BOSS-Gaussian interface for QM/MM simulations of Henry and methyl transfer reactions. *Journal of Computational Chemistry*, 36(27):2064–2074, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vikramaditya:2017:ARH

[VL17a] Talapunur Vikramaditya and Shiang-Tai Lin. Assessing the role of Hartree–Fock exchange, correlation energy and long range corrections in evaluating ionization potential, and electron affinity in density functional theory. *Journal of Computational Chemistry*, 38(21):1844–1852, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Volpi:2017:SCC

[VL17b] Riccardo Volpi and Mathieu Linares. Study of the cold charge transfer state separation at the TQ1/PC_{71} BM interface. *Journal of Computational Chemistry*, 38(14):1039–1048, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vikramaditya:2019:LGH

[VL19] Talapunur Vikramaditya and Shiang-Tai Lin. Limitations of global hybrids in predicting the geometries and torsional energy barriers of dimeric systems and the role of Hartree Fock and DFT exchange. *Journal of Computational Chemistry*, 40 (32):2810–2818, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valiente:2010:NPA

[VLB+10] Pedro A. Valiente, Alejandro Gil L., Paulo R. Batista, Ernesto R. Caffarena, Tirso Pons, and Pedro G. Pascutti. New parameterization approaches of the LIE method to improve free energy calculations of PlmII-inhibitors complexes. *Journal of Computational Chemistry*, 31(15):2723–2734, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vanLenthe:2012:LEE

[vLBBR12] J. H. van Lenthe, H. B. Broer-Braam, and Z. Rashid. Letters to the editor: On the efficiency of VBSCF algorithms, a comment on “An efficient algorithm for energy gradients and orbital optimization in valence bond theory”. *Journal of Computational Chemistry*, 33(8):911–913, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SSMW09].

Vines:2017:SSE

[VLGK+17] Francesc Viñes, Oriol Lamiel-García, Kyoung Chul Ko, Jin Yong Lee, and Francesc Illas. Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. *Journal of Computational Chemistry*, 38(11):781–789, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vorontsov:2011:CMD

[VM11] Ivan I. Vorontsov and Osamu Miyashita. Crystal molecular dynamics simulations to speed up MM/PB(GB)SA evaluation of binding free energies of di-mannose deoxy analogs with P51G-m4-Cyanovirin-N. *Journal of Computational Chemistry*, 32(6):1043–1053, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vreven:2019:CIF

[VM19] Thom Vreven and Stephen C. Miller. Computational investigation into the fluorescence of luciferin analogues. *Journal of*

Computational Chemistry, 40(2):527–531, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Villa:2017:CPA

[VMPS17] Francesco Villa, David Mignon, Savvas Polydorides, and Thomas Simonson. Comparing pairwise-additive and many-body generalized Born models for acid/base calculations and protein design. *Journal of Computational Chemistry*, 38(28): 2396–2410, October 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valdebenito-Maturana:2017:SNU

[VMRSH+17] Braulio Valdebenito-Maturana, Jose Antonio Reyes-Suarez, Jaime Henriquez, David S. Holmes, Raquel Quatrini, Ehmke Pohl, and Mauricio Arenas-Salinas. Software news and updates: Mutantelec: An in silico mutation simulation platform for comparative electrostatic potential profiling of proteins. *Journal of Computational Chemistry*, 38(7):467–474, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vohringer-Martinez:2010:RWP

[VMTL10] Esteban Vöhringer-Martinez and Alejandro Toro-Labbé. The role of water in the proton transfer reaction mechanism in tryptophan. *Journal of Computational Chemistry*, 31(14): 2642–2649, November 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2019:NHC

[VMV19] Arpita Varadwaj, Helder M. Marques, and Pradeep R. Varadwaj. Nature of halogen-centered intermolecular interactions in crystal growth and design: Fluorine-centered interactions in dimers in crystalline hexafluoropropylene as a prototype. *Journal of Computational Chemistry*, 40(20):1836–1860, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vorobjev:2010:BDM

[Vor10] Yury N. Vorobjev. Blind docking method combining search of low-resolution binding sites with ligand pose refinement by molecular dynamics-based global optimization. *Journal of Computational Chemistry*, 31(5):1080–1092, April 15, 2010.

CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vorobjev:2012:PMF

[Vor12] Yury N. Vorobjev. Potential of mean force of water–proton bath and molecular dynamic simulation of proteins at constant pH. *Journal of Computational Chemistry*, 33(8):832–842, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valdes:2019:QES

[VP19] Álvaro Valdés and Rita Prosmiti. Quantum effects on the stability of the He_5I_2 van der Waals conformers. *Journal of Computational Chemistry*, 40(25):2200–2206, September 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vchirawongkwin:2010:IQM

[VPR10] Viwat Vchirawongkwin, Andreas B. Pribil, and Bernd M. Rode. Ab initio quantum mechanical charge field study of hydrated bicarbonate ion: Structural and dynamical properties. *Journal of Computational Chemistry*, 31(2):249–257, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vanRijn:2019:QMS

[vRET19] Jeaphianne P. M. van Rijn, Andrés M. Escorcia, and Walter Thiel. QM/MM study of the taxadiene synthase mechanism. *Journal of Computational Chemistry*, 40(21):1902–1910, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vuori:2019:BGA

[VRKT19] Hannu T. Vuori, J. Mikko Rautiainen, Erkki T. Kolehmainen, and Heikki M. Tuononen. Benson group additivity values of phosphines and phosphine oxides: Fast and accurate computational thermochemistry of organophosphorus species. *Journal of Computational Chemistry*, 40(3):572–580, January 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vonRudorff:2017:CSP

[vRWGS17] Guido F. von Rudorff, Tobias Watermann, Xiang-Yang Guo, and Daniel Sebastiani. Conformational space of a polyphilic molecule with a fluorophilic side chain integrated in a DPPC bilayer. *Journal of Computational Chemistry*, 38(9):576–583, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vikramaditya:2014:ESB

[VS14] Talapunur Vikramaditya and Kanakamma Sumithra. Effect of substitutionally boron-doped single-walled semiconducting zigzag carbon nanotubes on ammonia adsorption. *Journal of Computational Chemistry*, 35(7):586–594, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vonSzentpaly:2018:ESP

[vS18] László von Szentpály. Eliminating symmetry problems in electronegativity equalization and correcting self-interaction errors in conceptual DFT. *Journal of Computational Chemistry*, 39(24):1949–1969, September 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vilseck:2011:OSF

[VSA11] Jonah Z. Vilseck, Somisetti V. Sambasivarao, and Orlando Acevedo. Optimal scaling factors for CM1 and CM3 atomic charges in RM1-based aqueous simulations. *Journal of Computational Chemistry*, 32(13):2836–2842, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venkatesan:2010:MDS

[VSD10] Santhosh Kannan Venkatesan, Anil Kumar Shukla, and Vikash Kumar Dubey. Molecular docking studies of selected tricyclic and quinone derivatives on trypanothione reductase of Leishmania infantum. *Journal of Computational Chemistry*, 31(13):2463–2475, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vanSeveren:2010:ATA

[vSGP10] Marie-Céline van Severen, Christophe Gourlaouen, and Olivier Parisel. Application of the topological analysis of the electronic localization function to archetypical [Pb(II)L_n]^p complexes: the bonding of Pb^{2+} revisited. *Journal of Computational Chemistry*, 31(1):185–194, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Voigt:2019:SDC

[VSH19] Bodo Alexander Voigt, Torben Steenbock, and Carmen Herrmann. Structural diradical character. *Journal of Computational Chemistry*, 40(7):854–865, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vincent:2019:APM

[VSP19] Mark A. Vincent, Arnaldo F. Silva, and Paul L. A. Popelier. Atomic partitioning of the MPn ($n = 2, 3, 4$) dynamic electron correlation energy by the interacting quantum atoms method: a fast and accurate electrostatic potential integral approach. *Journal of Computational Chemistry*, 40(32):2793–2800, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

VanDornshuld:2014:CPE

[VT14] Eric Van Dornshuld and Gregory S. Tschumper. Characterization of the potential energy surfaces of two small but challenging noncovalent dimers: $(P_2)_2$ and $(PCCP)_2$. *Journal of Computational Chemistry*, 35(6):479–487, March 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Viegas:2014:CCR

[VV14] Luís P. Viegas and António J. C. Varandas. Coupled-cluster reaction barriers of $HO_2 + H_2O + O_3$: an application of the coupled-cluster/Kohn–Sham density functional theory model chemistry. *Journal of Computational Chemistry*, 35(7):507–517, March 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vyboishchikov:2019:IAC

[VV19] Sergei F. Vyboishchikov and Alexander A. Voityuk. Iterative Atomic Charge Partitioning of Valence Electron Density. *Journal of Computational Chemistry*, 40(7):875–884, March 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanpoucke:2013:LER

[VVB13] Danny E. P. Vanpoucke, Isabel Van Driessche, and Patrick Bultinck. Letters to the Editor: Reply to 'Comment on "Extending Hirshfeld-I to bulk and periodic materials"'. *Journal of Computational Chemistry*, 34(5):422–427, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [VBV13a, Man13].

Vega-Vega:2017:MMC

[VVBL17] Álvaro Vega-Vega, Carmen Barrientos, and Antonio Largo. Metallic monoboronyl compounds: Prediction of their structure and comparison with the cyanide analogues. *Journal of Computational Chemistry*, 38(11):807–815, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Velez-Vega:2013:ODC

[VVG13] Camilo Velez-Vega and Michael K. Gilson. Overcoming dissipation in the calculation of standard binding free energies by ligand extraction. *Journal of Computational Chemistry*, 34 (27):2360–2371, October 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2015:HTM

[VVJ15] Pradeep R. Varadwaj, Arpita Varadwaj, and Bih-Yaw Jin. Hexahalogenated and their mixed benzene derivatives as prototypes for the understanding of halogen$\cdots$ halogen intramolecular interactions: New insights from combined DFT, QTAIM-, and RDG-based NCI analyses. *Journal of Computational Chemistry*, 36(31):2328–2343, December 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Visscher:2017:SAC

[VVLG17] Koen M. Visscher, C. Ruben Vosmeer, Rosa A. Luirink, and Daan P. Geerke. A systematic approach to calibrate a transferable polarizable force field parameter set for primary alcohols. *Journal of Computational Chemistry*, 38(8):508–517, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2018:HMD

[VVMY18] Pradeep R. Varadwaj, Arpita Varadwaj, Helder M. Marques, and Koichi Yamashita. Halogen in materials design: Chloroammonium lead triiodide perovskite ($ClNH_3PbI_3$) a dynamical bandgap semiconductor in 3D for photovoltaics. *Journal of Computational Chemistry*, 39(23):1902–1912, September 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2012:EST

[VVP12] Pradeep R. Varadwaj, Arpita Varadwaj, and Gilles H. Peslherbe. An electronic structure theory investigation of the physical chemistry of the intermolecular complexes of cyclopropenylidene with hydrogen halides. *Journal of Computational Chemistry*, 33(26):2073–2082, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vandewiele:2015:SCM

[VVV+15a] Nick M. Vandewiele, Ruben Van de Vijver, Kevin M. Van Geem, Marie-Françoise Reyniers, and Guy B. Marin. Symmetry calculation for molecules and transition states. *Journal of Computational Chemistry*, 36(3):181–192, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanduyfhuys:2015:SNU

[VVV+15b] Louis Vanduyfhuys, Steven Vandenbrande, Toon Verstraelen, Rochus Schmid, Michel Waroquier, and Veronique Van Speybroeck. Software news and updates: QuickFF: a program for a quick and easy derivation of force fields for metal-organic frameworks from ab initio input. *Journal of Computational Chemistry*, 36(13):1015–1027, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanduyfhuys:2018:EQF

[VVW+18] Louis Vanduyfhuys, Steven Vandenbrande, Jelle Wieme, Michel Waroquier, Toon Verstraelen, and Veronique Van Speybroeck. Extension of the QuickFF force field protocol for an improved accuracy of structural, vibrational, mechanical and thermal properties of metal-organic frameworks. *Journal of Computational Chemistry*, 39(16):999–1011, June 15,

2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2017:HOI

[VVY17] Arpita Varadwaj, Pradeep R. Varadwaj, and Koichi Yamashita. Hybrid organic–inorganic CH_3 NH_3 PbI_3 perovskite building blocks: Revealing ultra-strong hydrogen bonding and Mulliken inner complexes and their implications in materials design. *Journal of Computational Chemistry*, 38(32):2802–2818, December 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Varadwaj:2018:DSP

[VVY18] Arpita Varadwaj, Pradeep R. Varadwaj, and Koichi Yamashita. Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? Like attracting like! *Journal of Computational Chemistry*, 39(7): 343–350, March 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

vanWullen:2011:SMP

[vW11] Christoph van Wüllen. Shared-memory parallelization of the TURBOMOLE programs AOFORCE, ESCF, and EGRAD: How to quickly parallelize legacy code. *Journal of Computational Chemistry*, 32(6):1195–1201, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vyboishchikov:2015:MEE

[Vyb15] Sergei F. Vyboishchikov. Modeling exact exchange potential in spherically confined atoms. *Journal of Computational Chemistry*, 36(27):2037–2043, October 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vyboishchikov:2016:CEC

[Vyb16] Sergei F. Vyboishchikov. Correlation energy, correlated electron density, and exchange-correlation potential in some spherically confined atoms. *Journal of Computational Chemistry*, 37(31):2677–2686, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vanommeslaeghe:2015:RFM

[VYM15] Kenno Vanommeslaeghe, Mingjun Yang, and Alexander D. MacKerell Jr. Robustness in the fitting of molecular mechanics parameters. *Journal of Computational Chemistry*, 36(14): 1083–1101, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Voelz:2014:BIC

[VZ14] Vincent A. Voelz and Guangfeng Zhou. Bayesian inference of conformational state populations from computational models and sparse experimental observables. *Journal of Computational Chemistry*, 35(30):2215–2224, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weber:2017:IIR

[WAB17] Fabian Weber, Emad F. Aziz, and Annika Bande. Interdependence of ICD rates in paired quantum dots on geometry. *Journal of Computational Chemistry*, 38(25):2141–2150, September 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Walters:2017:DDD

[WAM17] Peter L. Walters, Thomas C. Allen, and Nancy Makri. Direct determination of discrete harmonic bath parameters from molecular dynamics simulations. *Journal of Computational Chemistry*, 38(2):110–115, January 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wei:2017:RSA

[WBF17] Shuai Wei, Charles L. Brooks III, and Aaron T. Frank. A rapid solvent accessible surface area estimator for coarse grained molecular simulations. *Journal of Computational Chemistry*, 38(15):1270–1274, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:RAN

[WBKS19] Yi-Gui Wang, Ericka C. Barnes, Savas Kaya, and Vinit Sharma. The reactivity of ambident nucleophiles: Marcus theory or hard and soft acids and bases principle? *Journal of Computational Chemistry*, 40(31):2761–2777, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wagner:2013:ATC

[WBN+13] Jeffrey R. Wagner, Gouthaman S. Balaraman, Michiel J. M. Niesen, Adrien B. Larsen, Abhinandan Jain, and Nagarajan Vaidehi. Advanced techniques for constrained internal coordinate molecular dynamics. *Journal of Computational Chemistry*, 34(11):904–914, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:CHE

[WBT10] Selina C. Wang, Peter A. Beal, and Dean J. Tantillo. Covalent hydration energies for purine analogs by quantum chemical methods. *Journal of Computational Chemistry*, 31(4):721–725, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2016:SGL

[WBVE16] Xiongwu Wu, Bernard R. Brooks, and Eric Vanden-Eijnden. Self-guided Langevin dynamics via generalized Langevin equation. *Journal of Computational Chemistry*, 37(6):595–601, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wan:2011:MDS

[WC11] Shunzhou Wan and Peter V. Coveney. Molecular dynamics simulation reveals structural and thermodynamic features of kinase activation by cancer mutations within the epidermal growth factor receptor. *Journal of Computational Chemistry*, 32(13):2843–2852, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2013:HWM

[WC13] Binju Wang and Zexing Cao. How water molecules modulate the hydration of CO_2 in water solution: Insight from the cluster-continuum model calculations. *Journal of Computational Chemistry*, 34(5):372–378, February 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wise:2014:NFF

[WC14] Olivia Wise and Orkid Coskuner. New force field parameters for metalloproteins I: Divalent copper ion centers including three histidine residues and an oxygen-ligated amino acid residue. *Journal of Computational Chemistry*, 35(17):1278–1289, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:QMS

[WCAH10] Hao Wu, Alana Canfield, Jhashanath Adhikari, and Shuanghong Huo. Quantum mechanical studies on model α-pleated sheets. *Journal of Computational Chemistry*, 31(6):1216–1223, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weill:2011:TCT

[WCDM11] Nathanael Weill, Christopher R. Corbeil, Joris W. De Schutter, and Nicolas Moitessier. Toward a computational tool predicting the stereochemical outcome of asymmetric reactions: Development of the molecular mechanics-based program ACE and application to asymmetric epoxidation reactions. *Journal of Computational Chemistry*, 32(13):2878–2889, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2014:SNU

[WCJ+14] Emilia L. Wu, Xi Cheng, Sunhwan Jo, Huan Rui, Kevin C. Song, Eder M. Dávila-Contreras, Yifei Qi, Jumin Lee, Viviana Monje-Galvan, Richard M. Venable, Jeffery B. Klauda, and Wonpil Im. Software news and updates: CHARMM–GUI Membrane Builder toward realistic biological membrane simulations. *Journal of Computational Chemistry*, 35(27):1997–2004, October 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2011:TSR

[WCL+11] Han-Ying Wu, Wan-Fei Cai, Lai-Cai Li, An-Min Tian, and Ning-Bew Wong. Theoretical study on the ring-opening isomerization reaction mechanism of the ring isomers of N_8H_8. *Journal of Computational Chemistry*, 32(12):2555–2563, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:IBF

[WCT+11] Fengting T. Wang, Lei Chen, Chuanjin J. Tian, Yan Meng, Zhigang G. Wang, Ruiqin Q. Zhang, Mingxing X. Jin, Ping Zhang, and Dajun J. Ding. Interactions between free radicals and a graphene fragment: Physical versus chemical bonding, charge transfer, and deformation. *Journal of Computational Chemistry*, 32(15):3264–3268, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Welborn:2015:WMS

[WCWV15] Matthew Welborn, Jiahao Chen, Lee-Ping Wang, and Troy Van Voorhis. Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. *Journal of Computational Chemistry*, 36(12):934–939, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:MMB

[WCWW11] Meiyan Wang, Lin Cheng, Jinping Wang, and Zhijian Wu. Mechanism of methylacetylene bisselenation catalyzed by palladium complex from density functional study. *Journal of Computational Chemistry*, 32(6):1170–1177, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:ELP

[WCY+11] Yin-Feng Wang, Wei Chen, Guang-Tao Yu, Zhi-Ru Li, Di Wu, and Chia-Chung Sun. Evolution of lone pair of excess electrons inside molecular cages with the deformation of the cage in e_2 @$C_{60}F_{60}$ systems. *Journal of Computational Chemistry*, 32(9):2012–2021, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wessel:2010:FPS

[WD10] Michael Wessel and Richard Dronskowski. A first-principles study on the existence and structures of the lighter alkaline-earth pernitrides. *Journal of Computational Chemistry*, 31(8): 1613–1617, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2013:PFB

[WDHZ13] Yao Wu, Xiaodong Dai, Niu Huang, and Lifeng Zhao. A partition function-based weighting scheme in force field parameter development using ab initio calculation results in global configurational space. *Journal of Computational Chemistry*, 34(15):1271–1282, June 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2019:BDA

[WDKT19] Xin Wu, Pavlo O. Dral, Axel Koslowski, and Walter Thiel. Big data analysis of ab Initio molecular integrals in the neglect of diatomic differential overlap approximation. *Journal of Computational Chemistry*, 40(4):638–649, February 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:DFT

[WDLG12] Fang Wang, Hong-Chen Du, Hui Liu, and Xue-Dong Gong. Density functional theory study of high-pressure effect on crystalline 4,4',6,6'-tetra(azido)hydrazo-1,3,5-triazine. *Journal of Computational Chemistry*, 33(22):1820–1830, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2012:QCI

[WDP+12] Qunyan Wu, Chunmei Deng, Qian Peng, Yingli Niu, and Zhigang Shuai. Quantum chemical insights into the aggregation induced emission phenomena: a QM/MM study for pyrazine derivatives. *Journal of Computational Chemistry*, 33(23):1862–1869, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:ABE

[WDS+19] Changwei Wang, David Danovich, Sason Shaik, Wei Wu, and Yirong Mo. Attraction between electrophilic caps: a counterintuitive case of noncovalent interactions. *Journal of Computational Chemistry*, 40(9):1015–1022, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wagener:2012:SNU

[WdVN12] Markus Wagener, Jacob de Vlieg, and Sander B. Nabuurs. Software news and updates: Flexible protein-ligand docking using the Fleksy protocol. *Journal of Computational Chemistry*, 33(12):1215–1217, May 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilson:2012:PHE

[WDW12] Brent R. Wilson, Nathan J. DeYonker, and Angela K. Wilson. Prediction of hydrocarbon enthalpies of formation by various thermochemical schemes. *Journal of Computational*

Chemistry, 33(25):2032–2042, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waller:2013:SNU

[WDY13] Mark P. Waller, Thomas Dresselhaus, and Jack Yang. Software news and updates: JACOB: an enterprise framework for computational chemistry. *Journal of Computational Chemistry*, 34(16):1420–1428, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2016:RMR

[WDZN16] Wei-Wei Wang, Jing-Shuang Dang, Xiang Zhao, and Shigeru Nagase. Regioselective multistep reconstructions of half-saturated zigzag carbon nanotubes. *Journal of Computational Chemistry*, 37(15):1363–1366, June 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weinhold:2012:NBO

[Wei12a] Frank Weinhold. Natural bond orbital analysis: a critical overview of relationships to alternative bonding perspectives. *Journal of Computational Chemistry*, 33(30):2363–2379, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weinhold:2012:SNU

[Wei12b] Frank Weinhold. Software news and updates: Natural bond critical point analysis: Quantitative relationships between natural bond orbital-based and QTAIM-based topological descriptors of chemical bonding. *Journal of Computational Chemistry*, 33(30):2440–2449, November 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Watanabe:2013:RDP

[WES13] Hiroshi Watanabe, Marcus Elstner, and Thomas Steinbrecher. Rotamer decomposition and protein dynamics: Efficiently analyzing dihedral populations from molecular dynamics. *Journal of Computational Chemistry*, 34(3):198–205, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weidlich:2016:SNU

[WF16] Iwona E. Weidlich and Igor V. Filippov. Software news and updates: Using the Gini coefficient to measure the chemical diversity of small-molecule libraries. *Journal of Computational Chemistry*, 37(22):2091–2097, August 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:AAC

[WFL+19] Qing Wang, Mingxing Fu, Xiaojun Li, Runfeng Huang, Rainer E. Glaser, and Lili Zhao. Aluminum alkoxy-catalyzed biomass conversion of glucose to 5-hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. *Journal of Computational Chemistry*, 40(16):1599–1608, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Warczinski:2019:ENA

[WFS19] Lisa Warczinski, Robert Franke, and Volker Staemmler. ESCAPE: a novel approach for a fast estimation of dynamic correlation energies: Application to large organic molecules. *Journal of Computational Chemistry*, 40(28):2491–2501, October 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2018:HHB

[WFZ+18] Changwei Wang, Yuzhuang Fu, Lina Zhang, David Danovich, Sason Shaik, and Yirong Mo. Hydrogen- and halogen-bonds between ions of like charges: Are they anti-electrostatic in nature? *Journal of Computational Chemistry*, 39(9):481–487, April 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wolf:2012:ENN

[WG12] Maarten G. Wolf and Gerrit Groenhof. Evaluating nonpolarizable nucleic acid force fields: a systematic comparison of the nucleobases hydration free energies and chloroform-to-water partition coefficients. *Journal of Computational Chemistry*, 33 (28):2225–2232, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wolf:2014:SNU

[WG14] Maarten G. Wolf and Gerrit Groenhof. Software news and updates: Explicit proton transfer in classical molecular dynamics simulations. *Journal of Computational Chemistry*, 35

(8):657–671, March 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wolanski:2018:CSZ

[WGA18] Lukasz Wolański, Dawid Grabarek, and Tadeusz Andruniów. Is the choice of a standard zeroth-order Hamiltonian in CASPT2 ansatz optimal in calculations of excitation energies in protonated and unprotonated Schiff bases of retinal? *Journal of Computational Chemistry*, 39(20):1470–1480, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2016:ODN

[WGD+16] Changwei Wang, Liangyu Guan, David Danovich, Sason Shaik, and Yirong Mo. The origins of the directionality of noncovalent intermolecular interactions. *Journal of Computational Chemistry*, 37(1):34–45, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:LHE

[WGL+11] Gui-Xiang Wang, Xue-Dong Gong, Yan Liu, Hong-Chen Du, Xiao-Juan Xu, and He-Ming Xiao. Looking for high energy density compounds applicable for propellant among the derivatives of DPO with N_3, ONO_2, and NNO_2 groups. *Journal of Computational Chemistry*, 32(5):943–952, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:ESH

[WGL12] Jing Wang, Jiande Gu, and Jerzy Leszczynski. The electronic spectra and the H-bonding pattern of the sulfur and selenium substituted guanines. *Journal of Computational Chemistry*, 33(19):1587–1593, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Witte:2016:ORC

[WGLG+16] Matthias Witte, Benjamin Grimm-Lebsanft, Arne Goos, Stephan Binder, Michael Rübhausen, Martin Bernard, Adam Neuba, Serge Gorelsky, Uwe Gerstmann, Gerald Henkel, Wolf Gero Schmidt, and Sonja Herres-Pawlis. Optical response of the Cu_2S_2 diamond core in $Cu2II(NGuaS)_2Cl_2$. *Journal of Computational Chemistry*, 37(24):2181–2192, September 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Witte:2016:DFT

[WGN+16] M. Witte, U. Gerstmann, A. Neuba, G. Henkel, and W. G. Schmidt. Density functional theory of the Cu_A-like Cu_2S_2 diamond core in $Cu_2II(NGuaS)_2Cl_2$. *Journal of Computational Chemistry*, 37(11):1005–1018, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:AMD

[WH11] Junmei Wang and Tingjun Hou. Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient. *Journal of Computational Chemistry*, 32 (16):3505–3519, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wolf:2010:GEI

[WHAS+10] Maarten G. Wolf, Martin Hoefling, Camilo Aponte-Santamaría, Helmut Grubmüller, and Gerrit Groenhof. `g_membed`: Efficient insertion of a membrane protein into an equilibrated lipid bilayer with minimal perturbation. *Journal of Computational Chemistry*, 31(11):2169–2174, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See erratum [WHAS+16].

Wolf:2016:ECG

[WHAS+16] Maarten G. Wolf, Martin Hoefling, Camilo Aponte-Santamaría, Helmut Grubmüller, and Gerrit Groenhof. Erratum: Corrigendum: `g_membed`: Efficient insertion of a membrane protein into an equilibrated lipid bilayer with minimal perturbation. *Journal of Computational Chemistry*, 37(21):2038, August 05, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [WHAS+10].

Wu:2011:TMS

[WHDL11] Nan-Nan Wu, Chao-Zheng He, Xue-Mei Duan, and Jing-Yao Liu. Theoretical mechanistic study on the reaction of CN radical with HNCN. *Journal of Computational Chemistry*, 32 (7):1449–1455, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Will:2013:SNU

[WHJH13] Thorsten Will, Michael C. Hutter, Johann Jauch, and Volkhard Helms. Software news and updates: Batch tautomer generation with MolTPC. *Journal of Computational Chemistry*, 34(28):2485–2492, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weymuth:2012:SNU

[WHK+12] Thomas Weymuth, Moritz P. Haag, Karin Kiewisch, Sandra Luber, Stephan Schenk, Christoph R. Jacob, Carmen Herrmann, Johannes Neugebauer, and Markus Reiher. Software news and updates: MoViPac: Vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. *Journal of Computational Chemistry*, 33 (27):2186–2198, October 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:TDD

[WHL+10] Rui Wang, Ce Hao, Peng Li, Ning-Ning Wei, Jingwen Chen, and Jieshan Qiu. Time-dependent density functional theory study on the electronic excited-state hydrogen-bonding dynamics of 4-aminophthalimide (4AP) in aqueous solution: 4AP and 4AP–$(H_2O)_{1,2}$ clusters. *Journal of Computational Chemistry*, 31(11):2157–2163, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiss:2010:GHO

[WHM10] Stewart N. Weiss, Lulu Huang, and Lou Massa. A generalized higher order kernel energy approximation method. *Journal of Computational Chemistry*, 31(16):2889–2899, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wei:2010:TDD

[WHX+10] Ning-Ning Wei, Ce Hao, Zhilong Xiu, Jingwen Chen, and Jieshan Qiu. Time-dependent density functional theory study on excited-state dihydrogen bonding OH$\cdots$HGe of the dihydrogen-bonded phenol-triethylgermanium complex. *Journal of Computational Chemistry*, 31(16):2853–2858, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2013:AEM

[WJG+13] Jia-Nan Wang, Jun-Ling Jin, Yun Geng, Shi-Ling Sun, Hong-Liang Xu, Ying-Hua Lu, and Zhong-Min Su. An accurate and efficient method to predict the electronic excitation energies of BODIPY fluorescent dyes. *Journal of Computational Chemistry*, 34(7):566–575, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:MND

[WJX+10] Yong Wu, Lu Jin, Ying Xue, Ik-Mo Lee, and Chan Kyung Kim. Mechanisms of norbornadiene dimerization to Binor-S using cationic Co^I, Rh^I, and Ir^I catalysts. *Journal of Computational Chemistry*, 31(12):2248–2257, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wadnerkar:2010:HUC

[WKC10a] Nitin Wadnerkar, Vijayanand Kalamse, and Ajay Chaudhari. Hydrogen uptake capacity of C_2H_4Sc and its ions: a density functional study. *Journal of Computational Chemistry*, 31(8): 1656–1661, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waldher:2010:FCF

[WKC+10b] Benjamin Waldher, Jadwiga Kuta, Samuel Chen, Neil Henson, and Aurora E. Clark. ForceFit: a code to fit classical force fields to quantum mechanical potential energy surfaces. *Journal of Computational Chemistry*, 31(12):2307–2316, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weng:2011:NPM

[WKC11] C. Weng, J. Kouvetakis, and A. V. G. Chizmeshya. A novel predictive model for formation enthalpies of Si and Ge hydrides with propane- and butane-like structures. *Journal of Computational Chemistry*, 32(5):835–853, April 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wadnerkar:2012:VDP

[WKLC12] Nitin Wadnerkar, Vijayanand Kalamse, Shyi-Long Lee, and Ajay Chaudhari. Verification of DFT-predicted hydrogen storage capacity of VC_3H_3 complex using molecular dynamics simulations. *Journal of Computational Chemistry*, 33(2):170–174, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:ALF

[WL10] Jun Wang and Ray Luo. Assessment of linear finite-difference Poisson–Boltzmann solvers. *Journal of Computational Chemistry*, 31(8):1689–1698, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Welsh:2014:ADF

[WL14] Ivan Welsh and Matthias Lein. Accurate density functional theory description of binding constants and NMR chemical shifts of weakly interacting complexes of C_{60} with corannulene-based molecular bowls. *Journal of Computational Chemistry*, 35(3):181–191, January 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:LPD

[WLC12] Shi-Bao Wang, Arvin Huang-Te Li, and Sheng D. Chao. Liquid properties of dimethyl ether from molecular dynamics simulations using ab initio force fields. *Journal of Computational Chemistry*, 33(9):998–1003, April 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wallnoefer:2011:CSF

[WLF11] Hannes G. Wallnoefer, Klaus R. Liedl, and Thomas Fox. A challenging system: Free energy prediction for factor Xa. *Journal of Computational Chemistry*, 32(8):1743–1752, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:MGC

[WLF19] Ya-Ting Wang, Xiang-Yang Liu, and Wei-Hai Fang. Mechanism of the O_2 ($^1\Delta_g$) generation from the Cl_2 /H_2O_2 basic aqueous solution explored by the combined ab initio calculation and nonadiabatic dynamics simulation. *Journal of Computational Chemistry*, 40(2):447–455, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:HAR

[WLHZ12] Li Wang, Yanjie Li, Hongqing He, and Jinglai Zhang. Hydrogen abstraction reactions of OH radicals with $CH_3CH_2CH_2Cl$ and $CH_3CHClCH_3$: a mechanistic and kinetic study. *Journal of Computational Chemistry*, 33(1):66–75, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2018:FBQ

[WLLH18] Yaqian Wang, Jinfeng Liu, Jinjin Li, and Xiao He. Fragment-based quantum mechanical calculation of protein-protein binding affinities. *Journal of Computational Chemistry*, 39 (21):1617–1628, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Witzke:2017:APP

[WLO+17] Sarah Witzke, Nanna Holmgaard List, Jógvan Magnus Haugaard Olsen, Casper Steinmann, Michael Petersen, Maarten T. P. Beerepoot, and Jacob Kongsted. An averaged polarizable potential for multiscale modeling in phospholipid membranes. *Journal of Computational Chemistry*, 38(9):601–611, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wei:2019:ESO

[WLQ19] Haixin Wei, Ray Luo, and Ruxi Qi. An efficient second-order Poisson–Boltzmann method. *Journal of Computational Chemistry*, 40(12):1257–1269, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:EET

[WLW+10] Yin-Feng Wang, Zhi-Ru Li, Di Wu, Chia-Chung Sun, and Feng-Long Gu. Excess electron is trapped in a large single molecular cage $C_{60}F_{60}$. *Journal of Computational Chemistry*, 31(1):195–203, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2012:LER

[WM12] Wei Wu and Yirong Mo. Letters to the editor: Reply to comment on the paper "An Efficient Algorithm for Energy Gradients and Orbital Optimization in Valence Bond Theory". *Journal of Computational Chemistry*, 33(8):914–915, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wuttke:2017:VDI

[WM17] Axel Wuttke and Ricardo A. Mata. Visualizing dispersion interactions through the use of local orbital spaces. *Journal of Computational Chemistry*, 38(1):15–23, January 05, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:SAG

[WMW+10] Jingheng Wu, Juan Mei, Sixiang Wen, Siyan Liao, Jincan Chen, and Yong Shen. A self-adaptive genetic algorithm-artificial neural network algorithm with leave-one-out cross validation for descriptor selection in QSAR study. *Journal of Computational Chemistry*, 31(10):1956–1968, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:TIE

[WMW11] Jing Wang, Jian Meng, and Zhijian Wu. Theoretical insights on the electron doping and Curie temperature in La-doped Sr_2CrWO_6. *Journal of Computational Chemistry*, 32(15):3313–3318, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ward:2017:EHR

[WNM17] Michael D. Ward, Shivangi Nangia, and Eric R. May. Evaluation of the hybrid resolution PACE model for the study of folding, insertion, and pore formation of membrane associated peptides. *Journal of Computational Chemistry*, 38(16):1462–1471, June 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2016:CPL

[WNP+16] Changhao Wang, Peter H. Nguyen, Kevin Pham, Danielle Huynh, Thanh-Binh Nancy Le, Hongli Wang, Pengyu Ren, and Ray Luo. Calculating protein–ligand binding affinities with MMPBSA: Method and error analysis. *Journal of Computational Chemistry*, 37(27):2436–2446, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiss:2015:ROS

[WO15] Alexander K. H. Weiss and Christian Ochsenfeld. A rigorous and optimized strategy for the evaluation of the Boys function kernel in molecular electronic structure theory. *Journal of Computational Chemistry*, 36(18):1390–1398, July 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2016:PHF

[WOH16] Ruixing Wang, Mikhail Ozhgibesov, and Hajime Hirao. Partial Hessian fitting for determining force constant parameters in molecular mechanics. *Journal of Computational Chemistry*, 37(26):2349–2359, October 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2018:AHF

[WOH18] Ruixing Wang, Mikhail Ozhgibesov, and Hajime Hirao. Analytical Hessian fitting schemes for efficient determination of force-constant parameters in molecular mechanics. *Journal of Computational Chemistry*, 39(6):307–318, March 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wong:2018:SMD

[Won18] Chung F. Wong. Steered molecular dynamics simulations for uncovering the molecular mechanisms of drug dissociation and for drug screening: a test on the focal adhesion kinase. *Journal of Computational Chemistry*, 39(19):1307–1318, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weidlich:2015:SNU

[WPM+15] Iwona E. Weidlich, Yuri Pevzner, Benjamin T. Miller, Igor V. Filippov, H. Lee Woodcock, and Bernard R. Brooks. Software news and updates: Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. *Journal of Computational Chemistry*, 36(1):62–67, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Witte:2017:CNO

[WRG+17] Matthias Witte, Martin Rohrmüller, Uwe Gerstmann, Gerald Henkel, Wolf Gero Schmidt, and Sonja Herres-Pawlis. $[Cu_6(NGuaS)_6]^{2+}$ and its oxidized and reduced derivatives: Confining electrons on a torus. *Journal of Computational Chemistry*, 38(20):1752–1761, July 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weijo:2010:WFP

[WRHF10] Ville Weijo, Maharavo Randrianarivony, Helmut Harbrecht, and Luca Frediani. Wavelet formulation of the polarizable continuum model. *Journal of Computational Chemistry*, 31 (7):1469–1477, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wessel:2012:EST

[WRM+12] C. Wessel, C. Reimann, A. Müller, D. Weber, M. Lerch, T. Ressler, T. Bredow, and R. Dronskowski. Electronic structure and thermodynamics of V_2O_3 polymorphs. *Journal of Computational Chemistry*, 33(26):2102–2107, October 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:IIC

[WS10] Chang-Sheng Wang and Chang-Liang Sun. Investigation on the individual contributions of N H$\cdots$O C and C H$\cdots$O C interactions to the binding energies of β-sheet models. *Journal of Computational Chemistry*, 31(5):1036–1044, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2011:CSR

[WS11] Chi-Shiun Wu and Ming-Der Su. A computational study of the reactivities of four-membered heavy carbene systems. *Journal of Computational Chemistry*, 32(9):1896–1906, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2012:TIR

[WS12] Chi-Shiun Wu and Ming-Der Su. Theoretical investigations of the reactivities of four-membered N-heterocyclic carbene analogues of the group 13 elements. *Journal of Computational Chemistry*, 33(1):103–111, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilkinson:2013:POG

[WS13] Karl Wilkinson and Chris-Kriton Skylaris. Porting ONETEP to graphical processing unit-based coprocessors. 1. FFT box operations. *Journal of Computational Chemistry*, 34(28): 2446–2459, October 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiser:2019:CBF

[WS19] Laura J. Weiser and Erik E. Santiso. A CGenFF-based force field for simulations of peptoids with both cis and trans peptide bonds. *Journal of Computational Chemistry*, 40(22): 1946–1956, August 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilkinson:2011:AGU

[WSGN11] Karl A. Wilkinson, Paul Sherwood, Martyn F. Guest, and Kevin J. Naidoo. Acceleration of the GAMESS-UK electronic structure package on graphical processing units. *Journal of Computational Chemistry*, 32(10):2313–2318, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2010:GTI

[WSH10] Ling Wang, Boris Stumm, and Volkhard Helms. Graph-theoretical identification of dissociation pathways on free energy landscapes of biomolecular interaction. *Journal of Computational Chemistry*, 31(4):847–854, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2019:EMK

[WSWD19] Yanze Wu, Huai Sun, Liang Wu, and Joshua D. Deetz. Extracting the mechanisms and kinetic models of complex reactions from atomistic simulation data. *Journal of Computational Chemistry*, 40(16):1586–1592, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2015:BCA

[WSZW15] Weizhou Wang, Tao Sun, Yu Zhang, and Yi-Bo Wang. Benchmark calculations of the adsorption of aromatic molecules on graphene. *Journal of Computational Chemistry*, 36(23):1763–1771, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:BBO

[WTD+19] Xiaohui Wang, Xingzhao Tu, Boming Deng, John Z. H. Zhang, and Zhaoxi Sun. BAR-based optimum adaptive steered MD for configurational sampling. *Journal of Computational Chemistry*, 40(12):1270–1289, May 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wirz:2016:SFG

[WTH+16] Lukas N. Wirz, Ralf Tonner, Andreas Hermann, Rebecca Sure, and Peter Schwerdtfeger. From small fullerenes to the graphene limit: a harmonic force-field method for fullerenes and a comparison to density functional calculations for Goldberg–Coxeter fullerenes up to C_{980}. *Journal of Computational Chemistry*, 37(1):10–17, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:CCN

[Wu10] Emilia L. Wu. Coriolis coupling and nonadiabaticity in chemical reaction dynamics. *Journal of Computational Chemistry*, 31(16):2827–2835, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weinhold:2014:BTH

[WvRSM14] Frank Weinhold, Paul von Ragué Schleyer, and William Chadwick McKee. Bay-type H···H "bonding" in cis-2-butene and related species: QTAIM versus NBO description. *Journal of Computational Chemistry*, 35(20):1499–1508, July 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2015:BCD

[WWCL15] Yi Wang, William Yi Wang, Long-Qing Chen, and Zi-Kui Liu. Bonding charge density from atomic perturbations. *Journal of Computational Chemistry*, 36(13):1008–1014, May 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wenzel:2014:CCL

[WWD14] Jan Wenzel, Michael Wormit, and Andreas Dreuw. Calculating core-level excitations and X-ray absorption spectra of medium-sized closed-shell molecules with the algebraic–diagrammatic construction scheme for the polarization propagator. *Journal of Computational Chemistry*, 35(26):1900–1915, October 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2011:MDS

[WWKS11] Yuhang Wang, Jason A. Wallace, Peter H. Koenig, and Jana K. Shen. Molecular dynamics simulations of ionic and nonionic surfactant micelles with a generalized Born implicit-solvent model. *Journal of Computational Chemistry*, 32(11): 2348–2358, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2016:BAS

[WWKS16] Hongyan Wang, Hui Wang, R. Bruce King, and Henry F. Schaefer III. Bis(azulene) “submarine” metal dimer sandwich compounds $(C_{10}H_8)_2$ M_2 (M = Ti, V, Cr, Mn, Fe, Co, Ni): Parallel and opposed orientations. *Journal of Computational Chemistry*, 37(2):250–260, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:MCA

[WWTL19] Yong-Heng Wang, An-An Wu, Kai Tan, and Xin Lu. Metal-catalyzed alkyne oxidation/C–H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. *Journal of Computational Chemistry*, 40(9):1038–1044, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:EPD

[WWU12] Jian Wang, Yu Wang, and Jesus M. Ugalde. Electron-pair density decomposition for core–valence separable systems. *Journal of Computational Chemistry*, 33(28):2243–2249, October 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:ULB

[WWW19] Dongdong Wang, Jingwei Weng, and Wenning Wang. An unconventional ligand-binding mechanism of substrate-binding proteins: MD simulation and Markov state model analysis of BtuF. *Journal of Computational Chemistry*, 40(14):1440–1448, May 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2018:BPN

[WWWW18] Bao Wang, Chengzhang Wang, Kedi Wu, and Guo-Wei Wei. Breaking the polar-nonpolar division in solvation free energy prediction. *Journal of Computational Chemistry*, 39(4):217–233, February 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2012:DCD

[WX12] Anan Wu and Xin Xu. DCMB that combines divide-and-conquer and mixed-basis set methods for accurate geometry optimizations, total energies, and vibrational frequencies of large molecules. *Journal of Computational Chemistry*, 33(16):1421–1432, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:SBC

[WXL$^+$12] Chengqi Wang, Lili Xi, Shuyan Li, Huanxiang Liu, and Xiaojun Yao. A sequence-based computational model for the prediction of the solvent accessible surface area for α-helix and β-barrel transmembrane residues. *Journal of Computational Chemistry*, 33(1):11–17, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2017:NIM

[WXL17] Changhao Wang, Li Xiao, and Ray Luo. Numerical interpretation of molecular surface field in dielectric modeling of solvation. *Journal of Computational Chemistry*, 38(14):1057–1070, May 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2012:EMA

[WXS$^+$12] Jia-Nan Wang, Hong-Liang Xu, Shi-Ling Sun, Ting Gao, Hong-Zhi Li, Hui Li, and Zhong-Min Su. An effective method for accurate prediction of the first hyperpolarizability of alkalides. *Journal of Computational Chemistry*, 33(2):231–236, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wong:2014:IPI

[WXY14] Kin-Yiu Wong, Yuqing Xu, and Darrin M. York. Ab initio path-integral calculations of kinetic and equilibrium isotope effects on base-catalyzed RNA transphosphorylation models. *Journal of Computational Chemistry*, 35(17):1302–1316, June 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2012:CDS

[WYGW12] Guangfen Wu, Mingli Yang, Xingyu Guo, and Jinlan Wang. Comparative DFT study of N_2 and no adsorption on vanadium clusters V_n ($n = 2$–13). *Journal of Computational Chemistry*, 33(23):1854–1861, September 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2015:DSW

[WYL$^+$15] Xiao Wang, Juan Yang, Ruoming Li, Hong Jiang, and Yan Li. Deformation of single-walled carbon nanotubes by interaction with graphene: a first-principles study. *Journal of Computational Chemistry*, 36(10):717–722, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2017:ARS

[WYT17] Chao Wang, Yizhong Yuan, and Xiaohui Tian. Assessment of range-separated exchange functionals and nonempirical functional tuning for calculating the static second hyperpolarizabilities of streptocyanines. *Journal of Computational Chemistry*, 38(9):594–600, April 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2017:ISD

[WZ17] Cheng Wang and Yingkai Zhang. Improving scoring-docking-screening powers of protein–ligand scoring functions using random forest. *Journal of Computational Chemistry*, 38(3):169–177, January 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2019:EUV

[WZ19] Yu-Chen Wang and Yi Zhao. Effect of an underdamped vibration with both diagonal and off-diagonal exciton-phonon interactions on excitation energy transfer. *Journal of Computational Chemistry*, 40(10):1097–1104, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:FPP

[wZbZ11] Chang wen Zhang and Fu bao Zheng. First-principles prediction on electronic and magnetic properties of hydrogenated AlN nanosheets. *Journal of Computational Chemistry*, 32(14): 3122–3128, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2019:TOS

[WZC+19] Yue Wu, Shengfu Zhang, Shuangshuang Cai, Xiong Xiao, Cheng Yin, Jian Xu, Shuxing Qiu, Wenzhou Yu, Meilong Hu, and Liangying Wen. Transformation of organic sulfur and its functional groups in Nantong and Laigang coal under microwave irradiation. *Journal of Computational Chemistry*, 40 (31):2749–2760, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2018:RLG

[WZH+18] Xue Wu, Si Zhou, Xiaoming Huang, Maodu Chen, R. Bruce King, and Jijun Zhao. Revisit of large-gap Si_{16} clusters encapsulating group-IV metal atoms (Ti, Zr, Hf). *Journal of Computational Chemistry*, 39(27):2268–2272, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2013:AEF

[WZK+13] Heng-Qing Wu, Rong-Lin Zhong, Yu-He Kan, Shi-Ling Sun, Min Zhang, Hong-Liang Xu, and Zhong-Min Su. After the electronic field: Structure, bonding, and the first hyperpolarizability of HArF. *Journal of Computational Chemistry*, 34 (11):952–957, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2010:TSC

[WZQW10] Xian-Hui Wu, Guo-Lin Zou, Jun-Min Quan, and Yun-Dong Wu. A theoretical study on the catalytic mechanism of Mus musculus adenosine deaminase. *Journal of Computational Chemistry*, 31(12):2238–2247, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2018:TPP

[WZWW18] Kedi Wu, Zhixiong Zhao, Renxiao Wang, and Guo-Wei Wei. Top P–S: Persistent homology-based multi-task deep neural networks for simultaneous predictions of partition coefficient and aqueous solubility. *Journal of Computational Chemistry*, 39(20):1444–1454, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2019:TSP

[XBSS19] Yang Xu, Peng Bao, Kai Song, and Qiang Shi. Theoretical study of proton coupled electron transfer reaction in the light state of the AppA BLUF photoreceptor. *Journal of Computational Chemistry*, 40(9):1005–1014, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2019:IBG

[XCLZ19] Xin Xu, Jun Chen, Shu Liu, and Dong H. Zhang. An ab initio-based global potential energy surface for the SH_3 system and full-dimensional state-to-state quantum dynamics study for the H_2 + HS → H_2 S + H reaction. *Journal of Computational Chemistry*, 40(10):1151–1160, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xi:2010:CMM

[XDL+10] Lili Xi, Juan Du, Shuyan Li, Jiazhong Li, Huanxiang Liu, and Xiaojun Yao. A combined molecular modeling study on gelatinases and their potent inhibitors. *Journal of Computational Chemistry*, 31(1):24–42, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2015:LSA

[XFG+15] Junchao Xia, William F. Flynn, Emilio Gallicchio, Bin W. Zhang, Peng He, Zhiqiang Tan, and Ronald M. Levy. Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. *Journal of Computational Chemistry*, 36(23):1772–1785, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2016:FAW

[XFG+16] Junchao Xia, William F. Flynn, Emilio Gallicchio, Bin W. Zhang, Peng He, Zhiqiang Tan, and Ronald M. Levy. The following articles were published in past issues of the *Journal of Computational Chemistry*: Large-scale asynchronous and distributed multidimensional replica exchange molecular simulations and efficiency analysis. *Journal of Computational Chemistry*, 37(6), March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2015:PHQ

[XFTW15] Kelin Xia, Xin Feng, Yiying Tong, and Guo Wei Wei. Persistent homology for the quantitative prediction of fullerene stability. *Journal of Computational Chemistry*, 36(6):408–422, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2016:QST

[XFX+16] Tianlv Xu, James Farrell, Yuning Xu, Roya Momen, Steven R. Kirk, Samantha Jenkins, and David J. Wales. QTAIM and stress tensor interpretation of the $(H_2O)_5$ potential energy surface. *Journal of Computational Chemistry*, 37(31):2712–2721, December 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2015:PPT

[XhD15] Jing Xu and Yi hong Ding. Pentaatomic planar tetracoordinate silicon with 14 valence electrons: a large-scale global search of $\mathrm{SiX}_n\mathrm{Y}_m^q$ ($n + m = 4$; $q = 0, \pm 1, -2$; X, Y = main group elements from H to Br). *Journal of Computational Chemistry*, 36(6):355–360, March 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xiao:2016:AEM

[XHLH16] Xingqing Xiao, Michelle E. Hung, Joshua N. Leonard, and Carol K. Hall. Adding energy minimization strategy to peptide-design algorithm enables better search for RNA-binding peptides: Redesigned λN peptide binds boxB RNA. *Journal of Computational Chemistry*, 37(27):2423–2435, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2018:LPS

[XKW18] Lihua Xu, Anshuman Kumar, and Bryan M. Wong. Linear polarizabilities and second hyperpolarizabilities of streptocyanines: Results from broken-symmetry DFT and new CCSD(T) benchmarks. *Journal of Computational Chemistry*, 39(28):2350–2359, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xue:2012:MMH

[XLY12] Weiwei Xue, Huanxiang Liu, and Xiaojun Yao. Molecular mechanism of HIV-1 integrase–vDNA interactions and strand transfer inhibitor action: a molecular modeling perspective. *Journal of Computational Chemistry*, 33(5):527–536, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xiong:2010:CDF

[XLYZ10] Ying Xiong, Junjun Liu, Guang-Fu Yang, and Chang-Guo Zhan. Computational determination of fundamental pathway and activation barriers for acetohydroxyacid synthase-catalyzed condensation reactions of α-keto acids. *Journal of Computational Chemistry*, 31(8):1592–1602, June 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2019:DHB

[XMA+19] Tianlv Xu, Roya Momen, Alireza Azizi, Tanja van Mourik, Herbert Früchtl, Steven R. Kirk, and Samantha Jenkins. The destabilization of hydrogen bonds in an external E-field for improved switch performance. *Journal of Computational Chemistry*, 40(21):1881–1891, August 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2015:SNU

[XML+15] Bing Xia, Artem Mamonov, Seppe Leysen, Karen N. Allen, Sergei V. Strelkov, Ioannis Ch. Paschalidis, Sandor Vajda, and Dima Kozakov. Software news and updates: Accounting for observed small angle X-ray scattering profile in the protein–protein docking server cluspro. *Journal of Computational Chemistry*, 36(20):1568–1572, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2016:STS

[XMSZ16] Xianjin Xu, Zhiwei Ma, Hongmin Sun, and Xiaoqin Zou. SM-TF: a structural database of small molecule-transcription factor complexes. *Journal of Computational Chemistry*, 37(17): 1559–1564, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xiang:2013:VBM

[XP13] Jin Yu Xiang and Jay W. Ponder. A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field. *Journal of Computational Chemistry*, 34(9): 739–749, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2011:FAC

[XSZL11] Beisi Xu, Hujun Shen, Xiao Zhu, and Guohui Li. Fast and accurate computation schemes for evaluating vibrational entropy of proteins. *Journal of Computational Chemistry*, 32 (15):3188–3193, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2011:MMD

[XTG+11] Bing Xia, Zheng-Fu Tai, Yu-Cheng Gu, Bang-Jing Li, Li-Sheng Ding, and Yan Zhou. MyMolDB: a micromolecular database solution with open source and free components. *Journal of Computational Chemistry*, 32(13):2942–2948, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2018:PLE

[XTn18] Enhua Xu and Seiichiro L. Ten-no. Partially linearized external models to active-space coupled-cluster through connected hextuple excitations. *Journal of Computational Chemistry*, 39 (15):875–880, June 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2014:IEP

[XTY+14] Fei Xia, Dudu Tong, Lifeng Yang, Dayong Wang, Steven C. H. Hoi, Patrice Koehl, and Lanyuan Lu. Identifying essential pairwise interactions in elastic network model using the alpha shape theory. *Journal of Computational Chemistry*, 35(15):

1111–1121, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2016:ACF

[XVA+16] You Xu, Kenno Vanommeslaeghe, Alexey Aleksandrov, Alexander D. MacKerell Jr., and Lennart Nilsson. Additive CHARMM force field for naturally occurring modified ribonucleotides. *Journal of Computational Chemistry*, 37(10):896–912, April 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2017:FEL

[XVN17] You Xu, Alessandra Villa, and Lennart Nilsson. The free energy of locking a ring: Changing a deoxyribonucleoside to a locked nucleic acid. *Journal of Computational Chemistry*, 38(15):1147–1157, June 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2015:MPB

[XW15] Kelin Xia and Guo-Wei Wei. Multidimensional persistence in biomolecular data. *Journal of Computational Chemistry*, 36(20):1502–1520, July 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2013:CPS

[XWSW13] Liang Xu, Xiaojuan Wang, Shengsheng Shan, and Xicheng Wang. Characterization of the polymorphic states of copper(II)-bound Aβ (1-16) peptides by computational simulations. *Journal of Computational Chemistry*, 34(29):2524–2536, November 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2011:QSS

[XWW+11] Jie Xu, Lei Wang, Luoxin Wang, Xiaolin Shen, and Weilin Xu. QSPR study of Setschenow constants of organic compounds using MLR, ANN, and SVM analyses. *Journal of Computational Chemistry*, 32(15):3241–3252, November 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2014:SMM

[XYW+14] Zhijun Xu, Yang Yang, Ziqiu Wang, Donald Mkhonto, Cheng Shang, Zhi-Pan Liu, Qiang Cui, and Nita Sahai. Small molecule-mediated control of hydroxyapatite growth: Free energy calculations benchmarked to density functional theory. *Journal of Computational Chemistry*, 35(1):70–81, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xie:2017:SNU

[XYX17] Yang Xie, Jinyong Ying, and Dexuan Xie. Software news and updates: SMPBS: Web server for computing biomolecular electrostatics using finite element solvers of size modified Poisson–Boltzmann equation. *Journal of Computational Chemistry*, 38(8):541–552, March 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2018:MIP

[XYZ18] Xianjin Xu, Chengfei Yan, and Xiaoqin Zou. MDockPeP: an ab-initio protein-peptide docking server. *Journal of Computational Chemistry*, 39(28):2409–2413, October 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xia:2011:AHE

[XZ11] Futing Xia and Hua Zhu. Alkaline hydrolysis of ethylene phosphate: an ab initio study by supermolecule model and polarizable continuum approach. *Journal of Computational Chemistry*, 32(12):2545–2554, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2011:DNS

[Yan11] Pei-Kun Yang. Discrepancy in the near-solute electric dipole moment calculated from the electric field. *Journal of Computational Chemistry*, 32(13):2783–2799, October 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2014:IES

[Yan14] Pei-Kun Yang. Incorporating the excluded solvent volume and surface charges for computing solvation free energy. *Journal of Computational Chemistry*, 35(1):62–69, January 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2016:EAS

[Yan16] Wei Yang. Editorial: Advanced sampling for molecular simulation is coming of age. *Journal of Computational Chemistry*, 37(6):549, March 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshii:2018:PTE

[YAO18] Noriyuki Yoshii, Yoshimichi Andoh, and Susumu Okazaki. Pressure tensor for electrostatic interaction calculated by fast multipole method with periodic boundary condition. *Journal of Computational Chemistry*, 39(19):1192–1199, July 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yap:2011:PDO

[Yap11] Chun Wei Yap. PaDEL-descriptor: an open source software to calculate molecular descriptors and fingerprints. *Journal of Computational Chemistry*, 32(7):1466–1474, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2013:CTS

[YAS13] Li Yang, Alauddin Ahmed, and Stanley I. Sandler. Comparison of two simulation methods to compute solvation free energies and partition coefficients. *Journal of Computational Chemistry*, 34(4):284–293, February 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2011:ETS

[YB11] Le Yu and Wensheng Bian. Extensive theoretical study on electronically excited states and predissociation mechanisms of sulfur monoxide including spin–orbit coupling. *Journal of Computational Chemistry*, 32(8):1577–1588, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamamoto:2013:TPM

[YB13] Shigeki Yamamoto and Petr Bouř. Transition polarizability model of induced resonance Raman optical activity. *Journal of Computational Chemistry*, 34(25):2152–2158, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yildiz:2016:AEK

[YB16] Dilan Yildiz and Uğur Bozkaya. Assessment of the extended Koopmans' theorem for the chemical reactivity: Accurate computations of chemical potentials, chemical hardnesses, and electrophilicity indices. *Journal of Computational Chemistry*, 37(3):345–353, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2019:GPL

[YBS19] Jinsol Yang, Minkyung Baek, and Chaok Seok. GalaxyDock3: Protein–ligand docking that considers the full ligand conformational flexibility. *Journal of Computational Chemistry*, 40 (31):2739–2748, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2010:TSN

[YCGA10] Guang Tao Yu, Wei Chen, Feng Long Gu, and Yuriko Aoki. Theoretical study on nonlinear optical properties of the Li^+ [calix[4]pyrrole]Li^- dimer, trimer and its polymer with diffuse excess electrons. *Journal of Computational Chemistry*, 31(4): 863–870, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Youn:2016:EEF

[YCK16] Il Seung Youn, Woo Jong Cho, and Kwang S. Kim. Effects of an electric field on interaction of aromatic systems. *Journal of Computational Chemistry*, 37(11):971–975, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2017:ERV

[YD17] Chong Yang and Andreas Dreuw. Evaluation of the restricted virtual space approximation in the algebraic-diagrammatic construction scheme for the polarization propagator to speed-up excited-state calculations. *Journal of Computational Chemistry*, 38(17):1528–1537, June 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2015:TPH

[YDGZ15] Kun Yuan, Jing-Shuang Dang, Yi-Jun Guo, and Xiang Zhao. Theoretical prediction of the host–guest interactions between novel photoresponsive nanorings and C_{60}: a strategy for facile encapsulation and release of fullerene. *Journal of Computational Chemistry*, 36(8):518–528, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yao:2010:SDS

[YDL+10] Yu-Hua Yao, Qi Dai, Ling Li, Xu-Ying Nan, Ping-An He, and Yao-Zhou Zhang. Similarity/dissimilarity studies of protein sequences based on a new 2D graphical representation. *Journal of Computational Chemistry*, 31(5):1045–1052, April 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2013:RWA

[YDR13] Jin Yang, Paul J. Dauenhauer, and Ashwin Ramasubramaniam. The role of water in the adsorption of oxygenated aromatics on Pt and Pd. *Journal of Computational Chemistry*, 34(1):60–66, January 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2016:PPA

[YDX16] Donghai Yu, Ruobing Du, and Ji-Chang Xiao. pK a prediction for acidic phosphorus-containing compounds using multiple linear regression with computational descriptors. *Journal of Computational Chemistry*, 37(18):1668–1671, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yesylevskyy:2012:SNU

[Yes12] Semen O. Yesylevskyy. Software news and updates: Pteros: Fast and easy to use open-source C++ library for molecular analysis. *Journal of Computational Chemistry*, 33(19):1632–1636, July 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yesylevskyy:2015:SNU

[Yes15] Semen O. Yesylevskyy. Software news and updates: Pteros 2.0: Evolution of the fast parallel molecular analysis library for C++ and Python. *Journal of Computational Chemistry*, 36(19):1480–1488, July 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2019:FSC

[YFH+19] Tao Yu, Florence Fabunmi, Jingsong Huang, Bobby G. Sumpter, and Jacek Jakowski. A fast scheme to calculate electronic couplings between P3HT polymer units using diabatic orbitals for charge transfer dynamics simulations. *Journal of Computational Chemistry*, 40(2):532–542, January 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2011:AMA

[YHCS11] Guangtao Yu, Xu-Ri Huang, Wei Chen, and Chia-Chung Sun. Alkali metal atom-aromatic ring: a novel interaction mode realizes large first hyperpolarizabilities of M@AR (M = Li, Na, and K, AR = pyrrole, indole, thiophene, and benzene). *Journal of Computational Chemistry*, 32(9):2005–2011, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2011:TSG

[YHG+11] Hua-Qing Yang, Chang-Wei Hu, Chao Gao, Meng-Yao Yang, Fang-Ming Li, Cai-Qin Li, and Xiang-Yuan Li. Theoretical study on the gas-phase reaction mechanism between palladium monoxide and methane. *Journal of Computational Chemistry*, 32(16):3440–3455, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2013:SNU

[YHH+13] Dong-Jun Yu, Jun Hu, Yan Huang, Hong-Bin Shen, Yong Qi, Zhen-Min Tang, and Jing-Yu Yang. Software news and updates: TargetATPsite: a template-free method for ATP-binding sites prediction with residue evolution image sparse representation and classifier ensemble. *Journal of Computational Chemistry*, 34(11):974–985, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2012:ECG

[YHVM12] Wenbo Yu, Xibing He, Kenno Vanommeslaeghe, and Alexander D. MacKerell Jr. Extension of the CHARMM general force field to sulfonyl-containing compounds and its utility in biomolecular simulations. *Journal of Computational Chemistry*, 33(31):2451–2468, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2017:PDS

[YHW17] Xiaojuan Yu, Hua Hou, and Baoshan Wang. Prediction on dielectric strength and boiling point of gaseous molecules for replacement of SF_6. *Journal of Computational Chemistry*, 38 (10):721–729, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2019:QDV

[YHX19] Dongzheng Yang, Xixi Hu, and Daiqian Xie. Quantum dynamics of vibration-vibration energy transfer for vibrationally excited HF colliding with H_2. *Journal of Computational Chemistry*, 40(10):1084–1090, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yeh:2011:DFT

[YJ11] Kuan-Yu Yeh and Michael J. Janik. Density functional theory-based electrochemical models for the oxygen reduction reaction: Comparison of modeling approaches for electric field and solvent effects. *Journal of Computational Chemistry*, 32 (16):3399–3408, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yourdkhani:2017:RPN

[YJ17] Sirous Yourdkhani and Mirosław Jabłoński. Revealing the physical nature and the strength of charge-inverted hydrogen bonds by SAPT(DFT), MP2, SCS-MP2, MP2C, and CCSD(T) methods. *Journal of Computational Chemistry*, 38 (11):773–780, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yourdkhani:2019:PNS

[YJ19] Sirous Yourdkhani and Mirosław Jabło'nski. Physical nature of silane$\cdots$carbene dimers revealed by state-of-the-art ab initio calculations. *Journal of Computational Chemistry*, 40(30): 2643–2652, November 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yakhanthip:2011:TIN

[YJN+11] Thanisorn Yakhanthip, Siriporn Jungsuttiwong, Supawadee Namuangruk, Nawee Kungwan, Vinich Promarak, Taweesak Sudyoadsuk, and Palita Kochpradist. Theoretical investigation of novel carbazole-fluorene based D-π-A conjugated organic dyes as dye-sensitizer in dye-sensitized solar cells (DSCs). *Journal of Computational Chemistry*, 32(8):1568–1576, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yao:2013:MDS

[YJXZ13] Xue X. Yao, Chang G. Ji, Dai Q. Xie, and John Z. H. Zhang. Molecular dynamics study of DNA binding by INT-DBD under a polarized force field. *Journal of Computational Chemistry*, 34(13):1136–1142, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamada:2013:VDE

[YK13] Kenta Yamada and Nobuaki Koga. Variationally determined electronic states for the theoretical analysis of intramolecular interaction. II. Qualitative nature of the P — O bond in phosphine oxides. *Journal of Computational Chemistry*, 34 (2):149–161, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2010:CSE

[YKH+10] Shihai Yan, Sunwoo Kang, Tomoyuki Hayashi, Shaul Mukamel, and Jin Yong Lee. Computational studies on electron and proton transfer in phenol-imidazole-base triads. *Journal of Computational Chemistry*, 31(2):393–402, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yourdkhani:2015:IBT

[YKH15] Sirous Yourdkhani, Tatiana Korona, and Nasser L. Hadipour. Interplay between tetrel and triel bonds in $RC_6H_4CN{\cdot}MF_3$ $CN{\cdot}BX_3$ complexes: a combined symmetry-adapted perturbation theory, Møller–Plesset, and quantum theory of atoms-in-molecules study. *Journal of Computational Chemistry*, 36 (32):2412–2428, December 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshikawa:2019:GAL

[YKNN19] Takeshi Yoshikawa, Nana Komoto, Yoshifumi Nishimura, and Hiromi Nakai. GPU-accelerated large-scale excited-state simulation based on divide-and-conquer time-dependent density-functional tight-binding. *Journal of Computational Chem-*

istry, 40(31):2778–2786, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamada:2011:TNA

[YKO+11] Kenta Yamada, Yoshiyuki Koyano, Takuya Okamoto, Toshio Asada, Nobuaki Koga, and Masataka Nagaoka. Toward a new approach for determination of solute's charge distribution to analyze interatomic electrostatic interactions in quantum mechanical/molecular mechanical simulations. *Journal of Computational Chemistry*, 32(14):3092–3104, November 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuzlenko:2013:MPN

[YL13] Olga Yuzlenko and Themis Lazaridis. Membrane protein native state discrimination by implicit membrane models. *Journal of Computational Chemistry*, 34(9):731–738, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2010:SPS

[YLCX10] Xue-Gang Yang, Wei Lv, Yu-Zong Chen, and Ying Xue. In silico prediction and screening of γ-secretase inhibitors by molecular descriptors and machine learning methods. *Journal of Computational Chemistry*, 31(6):1249–1258, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2014:GGA

[YLGX14] Xin Yan, Jiabo Li, Qiong Gu, and Jun Xu. gWEGA: GPU-accelerated WEGA for molecular superposition and shape comparison. *Journal of Computational Chemistry*, 35(15): 1122–1130, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yao:2011:BGB

[YLL11] Wen-Zhi Yao, Da-Zhi Li, and Si-Dian Li. Bridging gold: B-Au-B three-center–two-electron bonds in electron-deficient $B_2Au_n^{-/0}$ ($n = 1, 3, 5$) and mixed analogues. *Journal of Computational Chemistry*, 32(2):218–225, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2019:SIV

[YLS19] Yun-An Yan, Jian Liu, and Jiushu Shao. A semiclassical initial-value representation for quantum propagator and Boltzmann operator. *Journal of Computational Chemistry*, 40(10):1161–1171, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2019:FBQ

[YLT+19] Miao Yan, Hai-Ru Li, Xin-Xin Tian, Yue-Wen Mu, Hai-Gang Lu, and Si-Dian Li. Fluxional bonds in quasi-planar B_{18}^{2-} and half-sandwich MB_{18}^{-} (M = K, Rb, and Cs). *Journal of Computational Chemistry*, 40(11):1227–1232, April 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yin:2010:TDD

[YLZ+10] Shu-Hui Yin, Yufang Liu, Wei Zhang, Ming-Xing Guo, and Peng Song. Time-dependent density functional theory study on the hydrogen bonding-induced twisted intramolecular charge-transfer excited states of 2-(4'-N, N-dimethylaminophenyl)imidazo[4,5-b]pyridine. *Journal of Computational Chemistry*, 31(10):2056–2062, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2019:FBP

[YLZ+19] Miao Yan, Hai-Ru Li, Xiao-Yun Zhao, Xiao-Qin Lu, Yue-Wen Mu, Hai-Gang Lu, and Si-Dian Li. Fluxional Bonds in Planar B_{19}^{-}, Tubular Ta@B_{20}^{-}, and Cage-Like B_{39}^{-}. *Journal of Computational Chemistry*, 40(9):966–970, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2014:MEP

[YMP14] Yongna Yuan, Matthew J. L. Mills, and Paul L. A. Popelier. Multipolar electrostatics for proteins: Atom–atom electrostatic energies in crambin. *Journal of Computational Chemistry*, 35(5):343–359, February 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2019:CPB

[YMY+19] Wenhong Yang, Zhifeng Ma, Jun Yi, Sadia Ahmed, and Wen-Hua Sun. Catalytic performance of bis(imino)pyridine Fe/ Co complexes toward ethylene polymerization by 2D-/ 3D-QSPR modeling. *Journal of Computational Chemistry*, 40(13):1374–1386, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshikawa:2015:LSS

[YN15] Takeshi Yoshikawa and Hiromi Nakai. Linear-scaling self-consistent field calculations based on divide-and-conquer method using resolution-of-identity approximation on graphical processing units. *Journal of Computational Chemistry*, 36(3):164–170, January 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamaguchi:2017:RRA

[YNH+17] Shigeru Yamaguchi, Takahiro Nishimura, Yuta Hibe, Masaki Nagai, Hirofumi Sato, and Ian Johnston. Regularized regression analysis of digitized molecular structures in organic reactions for quantification of steric effects. *Journal of Computational Chemistry*, 38(21):1825–1833, August 5, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamauchi:2019:RSP

[YO19] Masataka Yamauchi and Hisashi Okumura. Replica sub-permutation method for molecular dynamics and Monte Carlo simulations. *Journal of Computational Chemistry*, 40(31): 2694–2711, December 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ou:2010:PMS

[yOaCG10] Yu yen Ou, Shu an Chen, and M. Michael Gromiha. Prediction of membrane spanning segments and topology in β-barrel membrane proteins at better accuracy. *Journal of Computational Chemistry*, 31(1):217–223, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamagishi:2014:NSA

[YOMT14] Junya Yamagishi, Noriaki Okimoto, Gentaro Morimoto, and Makoto Taiji. A new set of atomic radii for accurate estimation of solvation free energy by Poisson–Boltzmann solvent model. *Journal of Computational Chemistry*, 35(29):2132–2139, November 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yonezawa:2016:MPP

[Yon16] Yasushige Yonezawa. A method for predicting protein conformational pathways by using molecular dynamics simulations guided by difference distance matrices. *Journal of Computational Chemistry*, 37(13):1139–1146, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2016:DAS

[YOPB16] Xiaohu Yu, Artem R. Oganov, Ivan A. Popov, and Alexander I. Boldyrev. d-AO spherical aromaticity in Ce_6O_8. *Journal of Computational Chemistry*, 37(1):103–109, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohnishi:2016:ECF

[yOTn16] Yu ya Ohnishi and Seiichiro Ten-no. Explicitly correlated frequency-independent second-order Green's function for accurate ionization energies. *Journal of Computational Chemistry*, 37(27):2447–2453, October 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Youngs:2010:AAC

[You10] T. G. A. Youngs. Aten — an application for the creation, editing, and visualization of coordinates for glasses, liquids, crystals, and molecules. *Journal of Computational Chemistry*, 31 (3):639–648, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2010:TSF

[YPC+10] Kiyull Yang, Young Hee Park, Soo Gyeong Cho, Hai Whang Lee, Chan Kyung Kim, and Hyun-Joo Koo. Theoretical studies on the formation mechanism and explosive performance of nitro-substituted 1,3,5-triazines. *Journal of Computational Chemistry*, 31(13):2483–2492, October 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yesselman:2012:MAT

[YPKB12] Joseph D. Yesselman, Daniel J. Price, Jennifer L. Knight, and Charles L. Brooks III. MATCH: an atom-typing toolset for molecular mechanics force fields. *Journal of Computational Chemistry*, 33(2):189–202, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamada:2013:FPR

[YPvD13] Takahiro Yamada, Donald K. Phelps, and Adri C. T. van Duin. First principle and ReaxFF molecular dynamics investigations of formaldehyde dissociation on Fe(100) surface. *Journal of Computational Chemistry*, 34(23):1982–1996, September 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2013:FPS

[YR13] Rui Yang and Alistair P. Rendell. First principles study of gallium cleaning for hydrogen-contaminated α-Al_2O_3 (0001) surfaces. *Journal of Computational Chemistry*, 34(13):1101–1111, May 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2010:RPC

[YS10] Jia-Feng Yu and Xiao Sun. Reannotation of protein-coding genes based on an improved graphical representation of DNA sequence. *Journal of Computational Chemistry*, 31(11):2126–2135, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshizawa:2013:NSC

[YS13] Terutaka Yoshizawa and Shigeyoshi Sakaki. NMR shielding constants of CuX, AgX, and AuX (X = F, Cl, Br, and I) investigated by density functional theory based on the Douglas–Kroll–Hess Hamiltonian. *Journal of Computational Chemistry*, 34(12):1013–1023, May 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yosipof:2015:NNO

[YS15] Abraham Yosipof and Hanoch Senderowitz. k-Nearest neighbors optimization-based outlier removal. *Journal of Computational Chemistry*, 36(8):493–506, March 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yagi:2018:SMP

[YS18] Tomoaki Yagi and Hirofumi Sato. A simple model of planar membrane: an integral equation investigation. *Journal of Computational Chemistry*, 39(31):2576–2581, December 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2012:GAN

[YSG12] Keda Yang, Jiaye Su, and Hongxia Guo. GPU accelerated numerical simulations of viscoelastic phase separation model. *Journal of Computational Chemistry*, 33(18):1564–1571, July 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yousfi:2010:REM

[YSRSS10] N. Yousfi, M. Sekkal-Rahal, A. Sayede, and M. Springborg. Relaxed energetic maps of κ-carrabiose: a DFT study. *Journal of Computational Chemistry*, 31(6):1312–1320, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2012:MZE

[YSSB12] Hongfang Yang, Qisheng Song, Xinyu Song, and Yuxiang Bu. Multi-zinc-expanded graphene patches: Tetraradical versus diradical character. *Journal of Computational Chemistry*, 33 (21):1773–1780, August 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2012:IDC

[Yu12a] Feng Yu. Ab initio direct classical trajectory investigation on the S_N2 reaction of F^- with NH_2F: Nonstatistical central barrier recrossing dynamics. *Journal of Computational Chemistry*, 33(4):401–405, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2012:AIM

[Yu12b] Feng Yu. Assessment of ab initio MP2 and density functionals for characterizing the potential energy profiles of the S_N2 reactions at N center. *Journal of Computational Chemistry*, 33(15):1347–1352, June 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yanez:2017:FFG

[YVEI+17] Osvaldo Yañez, Alejandro Vásquez-Espinal, Diego Inostroza, Lina Ruiz, Ricardo Pino-Rios, and William Tiznado. A Fukui function-guided genetic algorithm. Assessment on structural prediction of Si_n (n = 12–20) clusters. *Journal of Computational Chemistry*, 38(19):1668–1677, July 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2012:ESL

[YW12] Yu Li Yan and Yuan Xu Wang. Electronic structure and low temperature thermoelectric properties of $In_{24}M_8O_{48}$ (M = Ge^{4+}, Sn^{4+}, Ti^{4+}, and Zr^{4+}). *Journal of Computational Chemistry*, 33(1):88–92, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2013:RNI

[YW13] Jack Yang and Mark P. Waller. Revealing noncovalent interactions in quantum crystallography: Taurine revisited. *Journal of Computational Chemistry*, 34(6):466–470, March 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2016:SNUa

[YWJ+16] Sheng-Chun Yang, Yong-Lei Wang, Gui-Sheng Jiao, Hu-Jun Qian, and Zhong-Yuan Lu. Software news and updates: Accelerating electrostatic interaction calculations with graphical processing units based on new developments of Ewald method using non-uniform Fast Fourier Transform. *Journal of Computational Chemistry*, 37(3):378–387, January 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2014:VSP

[YWZ14] Zhong-Zhi Yang, Jian-Jiang Wang, and Dong-Xia Zhao. Valence state parameters of all transition metal atoms in metalloproteins — development of ABEEM$\sigma\pi$ fluctuating charge force field. *Journal of Computational Chemistry*, 35(23):1690–1706, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2017:DSM

[YXZZ17] Haiyan Yuan, Pin Xiao, Yiying Zheng, and Jingping Zhang. DFT studies on the mechanism of Ag_2CO_3-catalyzed hydroazidation of unactivated terminal alkynes with TMS-N_3: an insight into the silver(I) activation mode. *Journal of Computational Chemistry*, 38(27):2289–2297, October 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2012:TSE

[YYT12] Xue-Fang Yu, Shohei Yamazaki, and Tetsuya Taketsugu. Theoretical study of the excited-state double proton transfer in the (3-methyl-7-azaindole)-(7-azaindole) heterodimer. *Journal of Computational Chemistry*, 33(20):1701–1708, July 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yan:2015:PPB

[YZ15a] Chengfei Yan and Xiaoqin Zou. Predicting peptide binding sites on protein surfaces by clustering chemical interactions. *Journal of Computational Chemistry*, 36(1):49–61, January 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2015:DHH

[YZ15b] Haiyan Yuan and Jingping Zhang. [DBU-H]$^+$ and H_2O as effective catalyst form for 2,3-dihydropyrido[2,3-d]pyrimidin-4(1H)-ones: a DFT study. *Journal of Computational Chemistry*, 36(17):1295–1303, June 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2016:EPC

[YZ16] Yuedong Yang and Yaoqi Zhou. Effective protein conformational sampling based on predicted torsion angles. *Journal of Computational Chemistry*, 37(11):976–980, April 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2017:MID

[YZ17] Haiyan Yuan and Jingping Zhang. Mechanistic insights on DBU catalyzed β-amination of NBS to chalcone driving by water: Multiple roles of water. *Journal of Computational Chemistry*, 38(7):438–445, March 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamabe:2014:DSP

[YZGS14a] Shinichi Yamabe, Guixiang Zeng, Wei Guan, and Shigeyoshi Sakaki. A DFT study on proton transfers in hydrolysis reactions of phosphate dianion and sulfate monoanion. *Journal of Computational Chemistry*, 35(30):2195–2204, November 15,

2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yamabe:2014:MCR

[YZGS14b] Shinichi Yamabe, Guixiang Zeng, Wei Guan, and Shigeyoshi Sakaki. S_N1–S_N2 and S_N2–S_N3 mechanistic changes revealed by transition states of the hydrolyses of benzyl chlorides and benzenesulfonyl chlorides. *Journal of Computational Chemistry*, 35(15):1140–1148, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2015:MDD

[YZL$^+$15] Haiyan Yuan, Yiying Zheng, Bo Li, Wenliang Li, and Jingping Zhang. The multieffects of DMF and DBU on the $[5 + 1]$ benzannulation of nitroethane and α-alkenoyl ketene-(S,S)-acetals: Hydrogen bonding and electrostatic interactions. *Journal of Computational Chemistry*, 36(10):731–738, April 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2018:MIW

[YZLZ18] Haiyan Yuan, Lihan Zhu, Wenliang Li, and Jingping Zhang. Mechanistic insight on water and substrate catalyzed the synthesis of 3-(1 H-indol-3-yl)-2-(4-methoxybenzyl)isoindolin-1-one: Driving by noncovalent interactions. *Journal of Computational Chemistry*, 39(27):2316–2323, October 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2019:ITD

[YZLZ19] Zhifang Yang, Yanping Zheng, Wenliang Li, and Jingping Zhang. Investigation of two-dimensional HF-based MXenes as the anode materials for Li/Na-ion batteries: a DFT study. *Journal of Computational Chemistry*, 40(13):1352–1359, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2013:DCS

[YZN13] Tao Yang, Xiang Zhao, and Shigeru Nagase. 1,3-dipolar cycloadditions of Stone–Wales defective single-walled carbon nanotubes: a theoretical study. *Journal of Computational Chemistry*, 34(26):2223–2232, October 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2011:IIZ

[YZWC11] Bo Yang, Yanyan Zhu, Yan Wang, and Guangju Chen. Interaction identification of Zif268 and $TATA_{ZF}$ proteins with GC-/AT-rich DNA sequence: a theoretical study. *Journal of Computational Chemistry*, 32(3):416–428, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2016:SNUb

[YZZ16] Yuedong Yang, Jian Zhan, and Yaoqi Zhou. Software news and updates: SPOT-Ligand: Fast and effective structure-based virtual screening by binding homology search according to ligand and receptor similarity. *Journal of Computational Chemistry*, 37(18):1734–1739, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2017:VWH

[YZZ+17] Kun Yuan, Rui-Sheng Zhao, Jia-Jia Zheng, Hong Zheng, Shigeru Nagase, Sheng-Dun Zhao, Yan-Zhi Liu, and Xiang Zhao. Van der Waals heterogeneous layer-layer carbon nanostructures involving $\pi\cdots$H-C-C-H$\cdots\pi\cdots$H-C-C-H stacking based on graphene and graphane sheets. *Journal of Computational Chemistry*, 38(10):730–739, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2015:DMM

[ZA15] Xun Zhu and Yuriko Aoki. Development of minimized mixing molecular orbital method for designing organic ferromagnets. *Journal of Computational Chemistry*, 36(16):1232–1239, June 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2018:ABD

[ZB18] Peiwen Zhao and Yuxiang Bu. Azobenzene-bridged diradical Janus nucleobases with photo-converted magnetic properties between antiferromagnetic and ferromagnetic couplings. *Journal of Computational Chemistry*, 39(20):1398–1405, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2016:NIC

[ZBB16] Yunfei Zhou, Xiaoguang Bao, and Weston Thatcher Borden. Nucleus-independent chemical shift analysis of the electronic states of the $(CO)_4$, $(CS)_4$, and $(CSe)_4$ molecules. *Journal of Computational Chemistry*, 37(1):46–48, January 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:DPP

[ZBG11] Peng Zhang, Peng Bao, and Jiali Gao. Dipole preserving and polarization consistent charges. *Journal of Computational Chemistry*, 32(10):2127–2139, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zierkiewicz:2015:TIH

[ZBMZH15] Wiktor Zierkiewicz, Dariusz C. Bieńko, Danuta Michalska, and Thérèse Zeegers-Huyskens. Theoretical investigation of the halogen bonded complexes between carbonyl bases and molecular chlorine. *Journal of Computational Chemistry*, 36 (11):821–832, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhong:2011:SPA

[ZBP11] Yang Zhong, Brad A. Bauer, and Sandeep Patel. Solvation properties of N-acetyl-β-glucosamine: Molecular dynamics study incorporating electrostatic polarization. *Journal of Computational Chemistry*, 32(16):3339–3353, December 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2014:REG

[ZC14] Weihong Zhang and Jianhan Chen. Replica exchange with guided annealing for accelerated sampling of disordered protein conformations. *Journal of Computational Chemistry*, 35 (23):1682–1689, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zoete:2011:SFF

[ZCGM11] Vincent Zoete, Michel A. Cuendet, Aurélien Grosdidier, and Olivier Michielin. SwissParam: a fast force field generation tool for small organic molecules. *Journal of Computational*

Chemistry, 32(11):2359–2368, August 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zabojnikova:2016:IPS

[ZCK+16] Tereza Zábojníková, Radim Cajzl, Jakob Kljun, Zdeněk Chval, Iztok Turel, and Jaroslav V. Burda. Interactions of the "piano-stool" [ruthenium(II)(η^6-arene)(quinolone)Cl]$^+$ complexes with water; DFT computational study. *Journal of Computational Chemistry*, 37(19):1766–1780, July 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2015:LVS

[ZCS+15] Shenggao Zhou, Li-Tien Cheng, Hui Sun, Jianwei Che, Joachim Dzubiella, Bo Li, and J. Andrew McCammon. LS–VISM: a software package for analysis of biomolecular solvation. *Journal of Computational Chemistry*, 36(14):1047–1059, May 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zou:2018:OLR

[ZCWX18] Wenli Zou, Ziyu Cai, Jiankang Wang, and Kunyu Xin. An open library of relativistic core electron density function for the QTAIM analysis with pseudopotentials. *Journal of Computational Chemistry*, 39(22):1697–1706, August 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2012:SNU

[ZDKM12] Ying Zhao, Antonio De Nicola, Toshihiro Kawakatsu, and Giuseppe Milano. Software news and updates: Hybrid particle-field molecular dynamics simulations: Parallelization and benchmarks. *Journal of Computational Chemistry*, 33(8):868–880, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2018:RPA

[ZDT18] Hongyu Zhou, Zheng Dong, and Peng Tao. Recognition of protein allosteric states and residues: Machine learning approaches. *Journal of Computational Chemistry*, 39(20):1481–1490, July 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zuvela:2018:IAB

[ZDW18] Petar Zuvela, Jonathan David, and Ming Wah Wong. Interpretation of ANN-based QSAR models for prediction of antioxidant activity of flavonoids. *Journal of Computational Chemistry*, 39(16):953–963, June 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2011:TDD

[ZDX11] Wenwei Zhao, Yihong Ding, and Qiying Xia. Time-dependent density functional theory study on the absorption spectrum of Coumarin 102 and its hydrogen-bonded complexes. *Journal of Computational Chemistry*, 32(3):545–553, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2013:NSR

[ZDZM13] Juan Zeng, LiLi Duan, John Z. H. Zhang, and Ye Mei. A numerically stable restrained electrostatic potential charge fitting method. *Journal of Computational Chemistry*, 34(10): 847–853, April 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:AIA

[ZFOS19] Yuqi Zhang, Stefano Forli, Anna Omelchenko, and Michel F. Sanner. AutoGridFR: Improvements on AutoDock affinity maps and associated software tools. *Journal of Computational Chemistry*, 40(32):2882–2886, December 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2018:FNC

[ZFS18] Xiaowang W. Zhou, Michael E. Foster, and Ryan B. Sills. An Fe-Ni-Cr embedded atom method potential for austenitic and ferritic systems. *Journal of Computational Chemistry*, 39 (29):2420–2431, November 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zubatyuk:2010:EDF

[ZGS+10] Roman I. Zubatyuk, Leonid Gorb, Oleg V. Shishkin, Mo Qasim, and Jerzy Leszczynski. Exploration of density functional methods for one-electron reduction potential of nitrobenzenes. *Journal of Computational Chemistry*, 31(1):144–

150, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2019:TSP

[ZGZ19] Qiuling Zhu, Xugeng Guo, and Jinglai Zhang. Theoretical study on photophysical properties of a series of functional pyrimidine-based organic light-emitting diodes emitters presenting thermally activated delayed fluorescence. *Journal of Computational Chemistry*, 40(16):1578–1585, June 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:CBU

[ZGZC19] Haomiao Zhang, Qiankun Gong, Haozhe Zhang, and Changjun Chen. Combining the biased and unbiased sampling strategy into one convenient free energy calculation method. *Journal of Computational Chemistry*, 40(20):1806–1815, July 30, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2012:CEE

[ZH12] Fangqiang Zhu and Gerhard Hummer. Convergence and error estimation in free energy calculations using the weighted histogram analysis method. *Journal of Computational Chemistry*, 33(4):453–465, February 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:SSE

[Zha11] Chaoyang Zhang. Shape and size effects in π–π interactions: Face-to-face dimers. *Journal of Computational Chemistry*, 32 (1):152–160, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:REFb

[Zha12a] Shuming Zhang. A reliable and efficient first principles-based method for predicting pK$_a$ values. 4. organic bases. *Journal of Computational Chemistry*, 33(31):2469–2482, December 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:REFa

[Zha12b] Shuming Zhang. A reliable and efficient first principles-based method for predicting pK$_a$ values. III. Adding explicit water molecules: Can the theoretical slope be reproduced and pK_a values predicted more accurately? *Journal of Computational Chemistry*, 33(5):517–526, February 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zou:2011:SSP

[ZHHX11] Dongsheng Zou, Zhongshi He, Jingyuan He, and Yuxian Xia. Supersecondary structure prediction using Chou's pseudo amino acid composition. *Journal of Computational Chemistry*, 32(2):271–278, January 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zanotto:2018:HPC

[ZHS+18] Leandro Zanotto, Gabriel Heerdt, Paulo C. T. Souza, Guido Araujo, and Munir S. Skaf. High performance collision cross section calculation — HPCCS. *Journal of Computational Chemistry*, 39(21):1675–1681, August 5, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zimmerman:2013:ADC

[Zim13] Paul M. Zimmerman. Automated discovery of chemically reasonable elementary reaction steps. *Journal of Computational Chemistry*, 34(16):1385–1392, June 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zimmerman:2015:SET

[Zim15] Paul M. Zimmerman. Single-ended transition state finding with the growing string method. *Journal of Computational Chemistry*, 36(9):601–611, April 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2013:FMS

[ZJZM13] Juan Zeng, Xiangyu Jia, John Z. H. Zhang, and Ye Mei. The F130L mutation in streptavidin reduces its binding affinity to biotin through electronic polarization effect. *Journal of Computational Chemistry*, 34(31):2677–2686, December 5, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2017:EGD

[ZKE+17] Baofeng Zhang, Denise Kilburg, Peter Eastman, Vijay S. Pande, and Emilio Gallicchio. Efficient Gaussian density formulation of volume and surface areas of macromolecules on graphical processing units. *Journal of Computational Chemistry*, 38(10):740–752, April 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2010:EES

[ZKH+10] Xiao Zhu, Peter Koenig, Michael Hoffmann, Arun Yethiraj, and Qiang Cui. Establishing effective simulation protocols for β- and α/β-peptides. III. Molecular mechanical model for acyclic β-amino acids. *Journal of Computational Chemistry*, 31(10):2063–2077, July 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:SGP

[ZL11] Changsheng Zhang and Luhua Lai. SDOCK: a global protein-protein docking program using stepwise force-field potentials. *Journal of Computational Chemistry*, 32(12):2598–2612, September 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2014:PCR

[ZLHH14] Panwang Zhou, Jianyong Liu, Keli Han, and Guozhong He. The photoisomerization of 11-cis-retinal protonated Schiff base in gas phase: Insight from spin-flip density functional theory. *Journal of Computational Chemistry*, 35(2):109–120, January 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2010:AFE

[ZLL+10] Laibin Zhang, Huifang Li, Jilai Li, Xiaohua Chen, and Yuxiang Bu. Absorption and fluorescence emission spectroscopic characters of naphtho-homologated yy-DNA bases and effect of methanol solution and base pairing. *Journal of Computational Chemistry*, 31(4):825–836, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2013:SNU

[ZLL+13] You-Liang Zhu, Hong Liu, Zhan-Wei Li, Hu-Jun Qian, Giuseppe Milano, and Zhong-Yuan Lu. Software news and updates: GALAMOST: GPU-accelerated large-scale molecular simulation toolkit. *Journal of Computational Chemistry*, 34(25):2197–2211, September 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:TSRb

[ZLLL12] Hui Zhang, Yang Liu, Jing-Yao Liu, and Ze-Sheng Li. Theoretical study and rate constants calculation for the reactions X + $CF_3CH_2OCF_3$ (X = F, Cl, Br). *Journal of Computational Chemistry*, 33(6):685–690, March 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2015:EMC

[ZLM+15] Liangxiao Zhang, Peiwu Li, Jin Mao, Fei Ma, Xiaoxia Ding, and Qi Zhang. An enhanced Monte Carlo outlier detection method. *Journal of Computational Chemistry*, 36(25):1902–1906, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2013:ICA

[ZLT13] Jian-Dong Zhang, Shu-Jin Li, and Fu-Ming Tao. Ab initio calculations of the Ar–ethane intermolecular potential energy surface using bond function basis sets. *Journal of Computational Chemistry*, 34(8):673–680, March 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2010:ITA

[ZLW10] Xiaoqi Zheng, Chun Li, and Jun Wang. An information-theoretic approach to the prediction of protein structural class. *Journal of Computational Chemistry*, 31(6):1201–1206, April 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2013:WPP

[ZLX+13] Mingyue Zheng, Yanlian Li, Bing Xiong, Hualiang Jiang, and Jingkang Shen. Water PMF for predicting the properties of water molecules in protein binding site. *Journal of Computational Chemistry*, 34(7):583–592, March 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2019:PRN

[ZLX+19] Yao-Xiao Zhao, Meng-Yang Li, Yi-Ming Xiong, Shirin Rahmani, Kun Yuan, Rui-Sheng Zhao, Masahiro Ehara, Shigeru Nagase, and Xiang Zhao. Pivotal role of nonmetal atoms in the stabilities, geometries, electronic structures, and isoelectronic chemistry of $Sc_3X@C_{80}$ (X = C, N, and O). *Journal of Computational Chemistry*, 40(31):2730–2738, December 5,

2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2016:LPT

[ZLY+16] Xue-Feng Zhao, Haixia Li, Cai-Xia Yuan, Yan-Qin Li, Yan-Bo Wu, and Zhi-Xiang Wang. Linear, planar, and tubular molecular structures constructed by double planar tetracoordinate carbon D_{2h} C_2 $(BeH)_4$ species via hydrogen-bridged BeH_2Be bonds. *Journal of Computational Chemistry*, 37(2): 261–269, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2014:ECM

[ZLZ14] Yi-Quan Zhang, Cheng-Lin Luo, and Qiang Zhang. Exchange coupling and magnetic anisotropy in a family of bipyrimidyl radical-bridged dilanthanide complexes: Density functional theory and ab initio calculations. *Journal of Computational Chemistry*, 35(12):904–909, May 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2010:PEF

[ZM10] Xiao Zhu and Alexander D. Mackerell Jr. Polarizable empirical force field for sulfur-containing compounds based on the classical Drude oscillator model. *Journal of Computational Chemistry*, 31(12):2330–2341, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zoboki:2011:ELN

[ZM11] T. Zoboki and I. Mayer. Extremely localized nonorthogonal orbitals by the pairing theorem. *Journal of Computational Chemistry*, 32(4):689–695, March 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:IRE

[ZMMM12] Hongjiang Zhang, Jean-Paul Malrieu, Haibo Ma, and Jing Ma. Implementation of renormalized excitonic method at ab initio level. *Journal of Computational Chemistry*, 33(1):34–43, January 5, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhong:2013:BST

[ZP13] Yang Zhong and Sandeep Patel. Binding structures of tri-N-acetyl-β-glucosamine in hen egg white lysozyme using molecular dynamics with a polarizable force field. *Journal of Computational Chemistry*, 34(3):163–174, January 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zerbetto:2014:LSF

[ZPF14] Mirco Zerbetto, Andrea Piserchia, and Diego Frezzato. Looking for some free energy? Call JEFREE (...). *Journal of Computational Chemistry*, 35(25):1865–1881, September 30, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zarycz:2016:CSB

[ZPP+16] Natalia Zarycz, Patricio F. Provasi, Gabriel I. Pagola, Marta B. Ferraro, Stefano Pelloni, and Paolo Lazzeretti. Computational study of basis set and electron correlation effects on anapole magnetizabilities of chiral molecules. *Journal of Computational Chemistry*, 37(17):1552–1558, June 30, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2014:TPC

[ZQ14] Hui Zhu and Zheng-Wang Qu. Toward product control in ring-opening oligomerization of 9H-9-borafluorenes. *Journal of Computational Chemistry*, 35(15):1107–1110, June 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:FTD

[ZQH19] Huan Zhang, Lili Qiu, and Dan Hu. Finite-temperature dimer method for finding saddle points on free energy surfaces. *Journal of Computational Chemistry*, 40(18):1701–1706, July 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zilberberg:2010:POD

[ZR10] Igor Zilberberg and Sergey Ruzankin. Paired orbitals for different spins equations. *Journal of Computational Chemistry*, 31(1):84–89, January 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zapata-Rivera:2011:ESR

[ZRCC11] Jhon Zapata-Rivera, Rosa Caballol, and Carmen J. Calzado. Electronic structure and relative stability of 1:1 Cu-O_2

adducts from difference-dedicated configuration interaction calculations. *Journal of Computational Chemistry*, 32(6): 1144–1158, April 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zapata-Rivera:2012:RML

[ZRCC12] Jhon Zapata-Rivera, Rosa Caballol, and Carmen J. Calzado. The role of macrocyclic ligands in the peroxo/superoxo nature of Ni–O_2 biomimetic complexes. *Journal of Computational Chemistry*, 33(16):1407–1415, June 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zgarbova:2015:TAD

[ZRL+15] Marie Zgarbová, Andreana M. Rosnik, F. Javier Luque, Carles Curutchet, and Petr Jurečka. Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. *Journal of Computational Chemistry*, 36(25):1874–1884, September 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zare-shahabadi:2010:AAC

[ZsA10] Vali Zare-shahabadi and Fatemeh Abbasitabar. Application of ant colony optimization in development of models for prediction of anti-HIV-1 activity of HEPT derivatives. *Journal of Computational Chemistry*, 31(12):2354–2362, September 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zadeh:2011:NAD

[ZSB+11] Joseph N. Zadeh, Conrad D. Steenberg, Justin S. Bois, Brian R. Wolfe, Marshall B. Pierce, Asif R. Khan, Robert M. Dirks, and Niles A. Pierce. NUPACK: Analysis and design of nucleic acid systems. *Journal of Computational Chemistry*, 32(1):170–173, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zoete:2016:ACD

[ZSB+16] Vincent Zoete, Thierry Schuepbach, Christophe Bovigny, Prasad Chaskar, Antoine Daina, Ute F. Röhrig, and Olivier Michielin. Attracting cavities for docking. Replacing the rough energy landscape of the protein by a smooth attracting landscape. *Journal of Computational Chemistry*, 37(4):437–

447, February 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2011:CDL

[ZSL+11] Li-Zhen Zhao, Wan-Sheng Su, Wen-Cai Lu, C. Z. Wang, and K. M. Ho. Competitive diamond-like and endohedral fullerene structures of Si_{70}. *Journal of Computational Chemistry*, 32 (7):1271–1278, May 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhan:2017:ASE

[ZSLL17] Xiaoling Zhan, Hu Shi, Hongguang Liu, and Jin Yong Lee. Applying strong external electric field to thiophene-based oligomers: a promising approach to upgrade semiconducting performance. *Journal of Computational Chemistry*, 38 (5):304–311, February 15, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2013:FPC

[ZSS+13] Yutong Zhao, Fu Kit Sheong, Jian Sun, Pedro Sander, and Xuhui Huang. A fast parallel clustering algorithm for molecular simulation trajectories. *Journal of Computational Chemistry*, 34(2):95–104, January 15, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zahariev:2014:FAM

[ZSTI14] Tsvetan K. Zahariev, Radomir I. Slavchov, Alia V. Tadjer, and Anela N. Ivanova. Fully atomistic molecular-mechanical model of liquid alkane oils: Computational validation. *Journal of Computational Chemistry*, 35(10):776–788, April 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zarate:2018:ERT

[ZSTRS+18] Ximena Zarate, Mario Saavedra-Torres, Angela Rodriguez-Serrano, Tatiana Gomez, and Eduardo Schott. Exploring the relevance of thiophene rings as bridge unit in acceptor-bridge-donor dyes on self-aggregation and performance in DSSCs. *Journal of Computational Chemistry*, 39(11):685–698, April 30, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:DFT

[ZSWL12] Riguang Zhang, Luzhi Song, Baojun Wang, and Zhong Li. A density functional theory investigation on the mechanism and kinetics of dimethyl carbonate formation on Cu_2O catalyst. *Journal of Computational Chemistry*, 33(11):1101–1110, April 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:FFD

[ZSYH12] Lu Zhang, Daniel-Adriano Silva, YiJing Yan, and Xuhui Huang. Force field development for cofactors in the photosystem II. *Journal of Computational Chemistry*, 33(25): 1969–1980, September 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2014:TSG

[ZSZ+14] Yunju Zhang, Jingyu Sun, Wanqiao Zhang, Yizhen Tang, and Rongshun Wang. Theoretical study on the gas phase reaction of propargyl alcohol with hydroxyl radical. *Journal of Computational Chemistry*, 35(22):1646–1656, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zinovjev:2014:ECR

[ZT14] Kirill Zinovjev and Iñaki Tuñón. Exploring chemical reactivity of complex systems with path-based coordinates: Role of the distance metric. *Journal of Computational Chemistry*, 35 (23):1672–1681, September 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zalesny:2015:TAD

[ZTH+15] Robert Zaleśny, Guangjun Tian, Christof Hättig, Wojciech Bartkowiak, and Hans Ågren. Toward assessment of density functionals for vibronic coupling in two-photon absorption: a case study of 4-nitroaniline. *Journal of Computational Chemistry*, 36(15):1124–1131, June 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zuev:2015:NAI

[ZVY+15] Dmitry Zuev, Eugene Vecharynski, Chao Yang, Natalie Orms, and Anna I. Krylov. New algorithms for iterative matrix-free eigensolvers in quantum chemistry. *Journal of Computational*

Chemistry, 36(5):273–284, February 15, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2017:BHH

[ZW17] Xiaojun Zhou and Fan Wang. Barrier heights of hydrogen-transfer reactions with diffusion quantum Monte Carlo method. *Journal of Computational Chemistry*, 38(11):798–806, April 30, 2017. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2018:YIB

[ZW18] Min Zheng and Mark P. Waller. Yoink: an interaction-based partitioning API. *Journal of Computational Chemistry*, 39 (13):799–806, May 15, 2018. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2015:ABO

[ZWF15] X. W. Zhou, D. K. Ward, and M. E. Foster. An analytical bond-order potential for carbon. *Journal of Computational Chemistry*, 36(23):1719–1735, September 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zaccaria:2016:IST

[ZWGO16] Francesco Zaccaria, Lando P. Wolters, Célia Fonseca Guerra, and Laura Orian. Insights on selenium and tellurium diaryldichalcogenides: a benchmark DFT study. *Journal of Computational Chemistry*, 37(18):1672–1680, July 5, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2013:MPI

[ZWL13] Xiaohua Zhang, Sergio E. Wong, and Felice C. Lightstone. Message passing interface and multithreading hybrid for parallel molecular docking of large databases on petascale high performance computing machines. *Journal of Computational Chemistry*, 34(11):915–927, April 30, 2013. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:ABD

[ZWLX11] Igor Ying Zhang, Jianming Wu, Yi Luo, and Xin Xu. Accurate bond dissociation enthalpies by using doubly hybrid XYG3 functional. *Journal of Computational Chemistry*, 32(9):1824–1838, July 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2010:PSM

[ZWMW10] Erjun Zhao, Jinping Wang, Jian Meng, and Zhijian Wu. Phase stability and mechanical properties of rhenium borides by first-principles calculations. *Journal of Computational Chemistry*, 31(9):1904–1910, July 15, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zadeh:2011:NAS

[ZWP11] Joseph N. Zadeh, Brian R. Wolfe, and Niles A. Pierce. Nucleic acid sequence design via efficient ensemble defect optimization. *Journal of Computational Chemistry*, 32(3):439–452, February 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2010:MDM

[ZWS+10] Xiaoyan Zheng, Xueye Wang, Keqi Shen, Nuanqing Wang, and Yueming Peng. Molecular design of a "molecular syringe" mimic for metal cations using a 1,3-alternate calix[4]arene cavity. *Journal of Computational Chemistry*, 31(11):2143–2156, August 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2010:SSP

[ZWW10] Erjun Zhao, Jinping Wang, and Zhijian Wu. Structural stability and phase transition in OsC and RuC. *Journal of Computational Chemistry*, 31(16):2883–2888, December 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2016:IBH

[ZWX16] Yuwei Zhou, Jianming Wu, and Xin Xu. Improving B3LYP heats of formation with three-dimensional molecular descriptors. *Journal of Computational Chemistry*, 37(13):1175–1190, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:AHF

[ZWX19] Igor Ying Zhang, Jianming Wu, and Xin Xu. Accurate heats of formation of polycyclic saturated hydrocarbons predicted by using the XYG3 type of doubly hybrid functionals. *Journal of Computational Chemistry*, 40(10):1113–1122, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2010:DFTb

[ZWY+10a] Xiaoyan Zheng, Xueye Wang, Shanfeng Yi, Nuanqing Wang, and Yueming Peng. Density functional theory study of calix[4]arene-*N*-azacrown-5, calix[4]arene-*N*-phenyl-azacrown-5, and their complexes with alkali-metal cations: Na^+, K^+, and Rb^+. *Journal of Computational Chemistry*, 31 (7):1458–1468, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2010:DFTa

[ZWY+10b] Xiaoyan Zheng, Xueye Wang, Shanfeng Yi, Nuanqing Wang, and Yueming Peng. Density functional theory study of the free and tetraprotonated spheroidal macrotricyclic ligands and the complexes with halide anions: F^-, Cl^-, Br^-. *Journal of Computational Chemistry*, 31(4):871–881, March 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2011:IIR

[ZWZ11] Chaoyang Zhang, Xiaolin Wang, and Mingfei Zhou. Isomers and isomerization reactions of four nitro derivatives of methane. *Journal of Computational Chemistry*, 32(8):1760–1768, June 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2011:HMM

[ZX11] Yongbing Zhao and Jingfa Xiao. Homology modeling and molecular dynamics simulation studies of human type 1 3β-hydroxysteroid dehydrogenase: Toward the understanding of cofactor specificity. *Journal of Computational Chemistry*, 32 (1):33–42, January 15, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:GCH

[ZX19] Ming-Xia Zhang and Hong-Liang Xu. A greener catalyst for hydroboration of imines-external electric field modify the reaction mechanism. *Journal of Computational Chemistry*, 40 (19):1772–1779, July 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2010:ESO

[ZXS+10] Yong Zhang, Wenhua Xu, Qiming Sun, Wenli Zou, and Wenjian Liu. Excited states of OsO_4: a comprehensive time-dependent relativistic density functional theory study. *Journal of Computational Chemistry*, 31(3):532–551, February 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2014:IDB

[ZY14] Dong-Xia Zhao and Zhong-Zhi Yang. Investigation of the distinction between van der Waals interaction and chemical bonding based on the PAEM-MO diagram. *Journal of Computational Chemistry*, 35(13):965–977, May 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2014:DSE

[ZYG+14] Pei Zhao, Tao Yang, Yi-Jun Guo, Jing-Shuang Dang, Xiang Zhao, and Shigeru Nagase. Dimetallic sulfide endohedral metallofullerene $Sc_2S@C_{76}$: Density functional theory characterization. *Journal of Computational Chemistry*, 35(22):1657–1663, August 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2015:TCS

[ZYG+15] Xu Zhang, Xiaodi Yang, Hua Geng, Guangjun Nan, Xingwen Sun, Jinyang Xi, and Xin Xu. Theoretical comparative studies on transport properties of pentacene, pentathienoacene, and 6,13-dichloropentacene. *Journal of Computational Chemistry*, 36(12):891–900, May 5, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2012:PPT

[ZYL+12] Weihua Zhu, Qingli Yan, Jinshan Li, Bibo Cheng, Yuling Shao, Xuelan Xia, and Heming Xiao. Prediction of the properties and thermodynamics of formation for energetic nitrogen-rich salts composed of triaminoguanidinium cation and 5-nitroiminotetrazolate-based anions. *Journal of Computational Chemistry*, 33(22):1781–1789, August 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:TSRa

[ZYLL12] Hui Zhang, Liu Yang, Jing-Yao Liu, and Ze-Sheng Li. Theoretical study on the reaction CX_3 + $SiH(CH_3)_3$ (X = H, F). *Journal of Computational Chemistry*, 33(2):203–210, January 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2015:PRM

[ZYR+15] Wen-Yang Zhao, Jie Yu, Si-Jia Ren, Xi-Guang Wei, Fang-Zhou Qiu, Peng-Hui Li, He Li, Yi-Peng Zhou, Chang-Zhen Yin, An-Pu Chen, Hao Li, Lei Zhang, Jun Zhu, Yi Ren, and Kai-Chung Lau. Probing the reactivity of microhydrated α-nucleophile in the anionic gas-phase S_N2 reaction. *Journal of Computational Chemistry*, 36(11):844–852, April 30, 2015. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2010:IAP

[ZYS+10] Lin Zhu, Jie Yang, Jiang-Ning Song, Kuo-Chen Chou, and Hong-Bin Shen. Improving the accuracy of predicting disulfide connectivity by feature selection. *Journal of Computational Chemistry*, 31(7):1478–1485, May 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2014:CBP

[ZYvIZ14] Huiying Zhao, Yuedong Yang, Mark von Itzstein, and Yaoqi Zhou. Carbohydrate-binding protein identification by coupling structural similarity searching with binding affinity prediction. *Journal of Computational Chemistry*, 35(30):2177–2183, November 15, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2016:CDO

[ZYW+16] Xue-Feng Zhao, Cai-Xia Yuan, Xiang Wang, Jia-Jia Li, Yan-Bo Wu, and Xiaotai Wang. Computational design of organometallic oligomers featuring 1,3-metal-carbon bonding and planar tetracoordinate carbon atoms. *Journal of Computational Chemistry*, 37(2):296–303, January 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2010:III

[ZZ10] Hao Zhang and Yun-Hong Zhang. Ab initio investigation on the ion-associated species and process in $Mg(NO_3\ )_2$ solution. *Journal of Computational Chemistry*, 31(15):2772–2782, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2012:CMF

[ZZ12] Cai-Hua Zhou and Xiang Zhao. Chemically modified fullerene derivatives as photosensitizers in photodynamic therapy: a first-principles study. *Journal of Computational Chemistry*, 33(8):861–867, March 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeller:2014:ECR

[ZZ14] Fabian Zeller and Martin Zacharias. Efficient calculation of relative binding free energies by umbrella sampling perturbation. *Journal of Computational Chemistry*, 35(31):2256–2262, December 5, 2014. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2010:TSRb

[ZZL+10a] Hui Zhang, Gui-Ling Zhang, Jing-Yao Liu, Miao Sun, Bo Liu, and Ze-Sheng Li. Theoretical studies on the reactions CH_3SCH_3 with OH, CF_3, and CH_3 radicals. *Journal of Computational Chemistry*, 31(15):2794–2803, November 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2010:TSRa

[ZZL+10b] Hui Zhang, Gui-Ling Zhang, Jing-Yao Liu, Miao Sun, Bo Liu, and Ze-Sheng Li. Theoretical study and rate constants calculation for the reactions of SiH_3 radical with SiH_3CH_3 and $SiH_2\ (CH_3\ )_2$. *Journal of Computational Chemistry*, 31(2): 403–411, January 30, 2010. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2012:AII

[ZZL+12] Yanli Zeng, Min Zhu, Xiaoyan Li, Shijun Zheng, and Lingpeng Meng. Assessment of intermolecular interactions at three sites of the arylalkyne in phenylacetylene-containing lithium-bonded complexes: ab initio and QTAIM studies. *Journal of*

Computational Chemistry, 33(14):1321–1327, May 30, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2019:STE

[ZZL19] ZhiYe Zhu, Yi Zhao, and WanZhen Liang. Singlet/ triplet exciton dissociation and charge recombination in donor-acceptor ThQs-C_{60} /PDIxCN_2 complexes. *Journal of Computational Chemistry*, 40(9):997–1004, April 5, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2019:PVM

[ZZMW19] Huaiyu Zhang, Chen Zhou, Yirong Mo, and Wei Wu. Performance of the VBSCF method for pericyclic and π bond shift reactions. *Journal of Computational Chemistry*, 40(10):1123–1129, April 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2012:RMC

[ZZWT12] Wenjing Zhang, Yanyan Zhu, Donghui Wei, and Mingsheng Tang. Reviews: Mechanisms of the cascade synthesis of substituted 4-amino-1,2,4-triazol-3-one from huisgen zwitterion and aldehyde hydrazone: a DFT study. *Journal of Computational Chemistry*, 33(7):715–722, March 15, 2012. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2011:CSE

[ZZWX11] Weihua Zhu, Chenchen Zhang, Tao Wei, and Heming Xiao. Computational study of energetic nitrogen-rich derivatives of 1,1'- and 5,5'-bridged ditetrazoles. *Journal of Computational Chemistry*, 32(10):2298–2312, July 30, 2011. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2016:CQD

[ZZY+16] Xin Zhang, Yuan Zhao, Honggao Yan, Zexing Cao, and Yirong Mo. Combined QM(DFT)/ MM molecular dynamics simulations of the deamination of cytosine by yeast cytosine deaminase (yCD). *Journal of Computational Chemistry*, 37(13):1163–1174, May 15, 2016. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2019:ISO

[ZZZ+19] Changyan Zhu, Xingxing Zhang, Min Zhang, Yun Geng, Xingman Liu, and Zhongmin Su. Insight into spin-orbital interaction using MCSCF method: a special analysis of the $^1\Sigma_g^+$ electronic state in C_2 and the linear polyacetylenic C_4 and C_6. *Journal of Computational Chemistry*, 40(13):1338–1343, May 15, 2019. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).