A Complete Bibliography of Publications in *Journal of Computational Chemistry*: 2020–2029

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Title word cross-reference

[GKA+23b]. [**?**]KohnEhlert:2020:PPP. **-lactamase** [KGD+21]. **-LIO** [SDK20]. **-matrix** [WHJM23]. **-methylide** [SVTK+22]. **-modified** [DOT22]. **-octanol-water** [SHH+23b]. **-phenyl** [AS20]. **-pyrazine-M** [MH20]. **-pyrido** [MIP+22]. **-pyrrolylenones** [ARR22b]. **-radical** [MP23]. **-sextet** [TLD+22]. **-sheets** [XIV+24]. **-thymine** [SSS+20a]. **-TriPip222** [Ari24]. **-water** [VCRP23]. **-xTB** [OM22].

/CBS [CSWW20, Dor20, SK20]. **/H** [WSV20]. **/N** [ZHG+24].

1 [CM20b, CBK+24, KUNT20, PWX+20, Sán20, WCT+23]. **1-** [MLGY24]. **1-11** [ZDBZ20]. **1-chloro-3** [BR23]. **1.0** [Che23, XSP+23]. **1.2-a** [MIP+22]. **10.1002/jcc.25747** [MT20a]. **12** [SMH21]. **1233zd** [BR23]. **1234yf** [BR23]. **19** [SLMA21].

2 [BBBP+23, MSE+21, dMBdAVdS24, CM20b, EIT+21, GCP22, KLZ+23, KGD+21, ONA+20, PDC23, PPP21, PPRS22, RLR+20, SLR+20, UAC+23, YC23]. **2'-bipyridyl** [BBBP+23]. **2-body** [KG23]. **2'-disulfanediylbis** [MSE+21]. **2-ethenediol** [MLGY24]. **2-ethylhexanoate** [BR23]. **2-HOPO** [SDK20]. **2-hydroxymethyl** [MSA22a]. **2-methoxyethyl** [MSA22a]. **2-siloxy-1-propene** [LLS+22b]. **2.0** [FPMD23, Kos22, SWLC22]. **20/HMX** [ZG21]. **2D** [POPGS22, PM21]. **2D-surface** [PM21]. **2D/3D** [POPGS22].

3 [BBBP+23, GSJ+23, VZG+24]. **3-cycloaddition** [SVTK+22]. **3-D** [GSJ+23]. **3-dienes** [BXY+24]. **3-tetrafluoro-1-propene** [BR23]. **3-trifluoro-1-nitroprop-1-ene** [SMB+23]. **3-trifluoropropene** [BR23]. **31** [dSSRVdM24]. **3D** [CKH23, DF22, HKFT21, POPGS22, YIO20, YYZ+21]. **3D-COF** [YYZ+21]. **3D-QSAR** [DF22, HKFT21]. **3D-QSAR/MD** [HKFT21]. **3D-RISM** [CKH23, MY24, YIO20].

4-oxo-4 [MIP+22]. **4-triazole-3-thione** [KGD+21]. **40** [MT20a]. **42** [WG21]. **43** [SCCZ21]. **4polyGraft** [Che23].

6 [BTC24]. **6-dimethylfulvene** [SHH+24]. **6-hydroxyquinolinone** [SEBE21]. **6-lutidine** [TYZ20]. **60th** [IBL20]. **66** [FP23].

7 [CM20b]. **74** [ZHG+24]. **7D** [Bal20a]. **7D-Hypercube** [Bal20a].

8-hydroxyquinolinato [AS20].

= [AQRA+23, AQMM+23, AQIS+24, ABAQ+23, AS20, APR21, GPM21b, HSG21, LZW+23, LXP+22, LWC+24, LJW+23, MH20, PTP23, PP23, SS24, SM22b, SCC+22, SL20, WTST24a, WZW+24, ZDBZ20].

AA [ZWY+22]. **Ab-Initio**

[SHH+23b, UKBD23]. **coefficients** [BUNO22b]. **Coelenterazine** [GOY20]. **Coenzyme** [CWZD20]. **COF** [YYZ+21]. **coherent** [EVKL21]. **coinage** [FBM+23, MCD22, YSMS24]. **Colab** [PSW+24]. **coli** [CGSP24a]. **collective** [BPT+23]. **collective-variable** [BPT+23]. **collision** [BBY+21]. **Colorings** [Bal20a]. **combination** [GVJ+22, KK23]. **Combined** [RMJ21, AiIS+21, KPHV23, LDT+22, TIK21, TMO+21, WKD+21]. **Combining** [BMT+21, MKB+21, TCS+21a, WSL+20, KN21, NML21]. **Comment** [MT21, NTK21, WFLZ23, WG21, CPG21, Wan21a]. **common** [MSA22a]. **communications** [AiIS+21]. **Comparative** [JMV21, PM21, BA24, SGRN24, THH+24]. **compared** [LML+23, WD20]. **Comparing** [CCHS23]. **Comparison** [BSS+22, CN21, NUK21, RLHG+23, SK20, WK21, Ano24a, DGM22, GG22, HSG21, SVTK+22, SK23]. **compatible** [BTL24, PLP+20]. **competing** [ĆNF23]. **competition** [SJZ+21]. **complementary** [FPMD23, SM22a]. **Complete** [HL20, DMD+21, MCP23, SCKH21]. **Complex** [NGD22, ALA20, AAL21, BF22, GNK+23, KL20, LML+23, Mon24, OE20, SWF+20, SIW21, SC23, TM20, WHJM23, YYS20, ZMH+21, ZZG+21]. **complexation** [SGRN24, SDK20]. **Complexes** [AD20, BGS+20, ASL+20, AS23, AS20, Ari24, BKM21, Brz22, CL23, CMD+22, ĆPP+22, DGM22, DSK21, FNPD22, GKA+23b, GP21, Jab22a, KMR+24, KK23, KBHG23, KKAK23, KDP+22, LLKS23, LKT21, LZW+23, LML+23, MNH21, MVP+20, MLM+24, MGB+22, MYYS24, MCD22, NBE+23, PTP23, PB20, PLT24, PP23, RLHG+23, SVDS21, SEZ20, SD21, THLC+23, WYC+24, XZX+22, YFS20, YSMS24, dBCdL20]. **component** [IWN24, KWYN23, KL20]. **components** [AV20, NTK21]. **composite** [CK22, PW20, PCB+24, SFS24]. **composites** [MML+23]. **Composition** [YLZ+22, JS21]. **Composition-selective** [YLZ+22]. **compound** [EK20b, HTFY21, QLW+22b, SWM+20b]. **compound-protein** [QLW+22b]. **Compounds** [PAS+20, SL20, BW22a, dMBdAVdS24, KBK+24, MAI22, MCP23, MP23, NI22, NPGP23, PDGD22, PDGD23, PHS+20, QLW+22b, SW21, SS24]. **Comprehensive** [SS24, YIO20, JGdC+23, PRH20, ZK23]. **compressed** [XZZ+20]. **compression** [CC22]. **Comput** [MT20a, WG21]. **Computation** [ALA20, CM20a, GZFSM21, MN20, SZL23]. **Computational** [ARA22, AD20, AR20, BW22a, ĆNF23, GOY20, KZP22, KMR+24, KJV23, KBHG23, MPV22, Sai23, SKGG23, XZ20, ZMH+21, CGSP24a, CBK+24, CRT+21, DSS+24, JC20, KZJ22, KPHV23, LCP21, MDO+20, MK22a, MSA22b, NMMC21, Ore24, PSGL21, SW21, SVDS21, SBB+22, TTH+21a, VAP+21, WG20]. **Computationally** [ZBH+23, TPD21]. **Computations** [Bal20a, Bal20b, BSF20, RBM+23]. **compute** [SYS+21]. **computed** [MEKH22, MM24, ZWR22]. **Computer** [KGS+22]. **Computer-aided** [KGS+22]. **Computing** [GJMPVR+20, IRB+23, JKK+21, KWMPR24b, MPP23, POvG21]. **concentrations** [CX21b]. **conceptual** [ĆPP+22, GD23, MGCM21].

Drude [BS23, KLP+22, KYM20, LJ20, ODL20]. **Drug** [SLMA21, AAID22, CBK+24, DYGM21, HKFT21, LSP23, RKC21, RDK+22, SSPK24]. **drug-delivery** [AAID22]. **drug-like** [DYGM21]. **druglike** [SHH+23b]. **drugs** [HS22, HS23, HBM+20, KMR+24, NST+20, PRH20, dCRM21]. **Dual** [YW20, MPP23]. **dual-atom** [DLH+23]. **Dual-hybrid** [YW20]. **due** [FBP+22, MAM21, ÖLP+20, SSPK24]. **dyes** [TMO+21]. **dynamic** [BAO+20, BBBP+23, IAS+24, MPOC21, MK22a, PCB+24, SYS+21]. **dynamical** [RR22, SZL23]. **dynamically** [MT20b, TWT+22]. **Dynamics** [FMFG20, HHL+20, KUNT20, YXGZ20, Zac20, AiIS+21, ALA+22, BUNO22b, BAO+20, BR23, BTL24, BBL+22, CDCT21, CSP20, CST23, CCPR24, DHN+21, FMK24, FNY21, FBP+22, GGK20, GK24, GG22, JRS20, JKK+21, KR23, KOD21, KLP+22, LL21a, LKM20, LHH+21, LEP+21, MN20, MKK+22, MGB+22, MSA22a, MAP+20, NLC23, Nan24, NN20, NP23, OSHT20, PBM21, PDL+21, POvG21, PGP+23, PPP21, PM21, QLC+20, RKC21, RDK+22, RGGD21, RPD+20a, SPSH20, Shi22, SY21, SWLC22, SCC+22, SSPK24, SSFS22b, SKKK20, SCCZ21, TPB22, UKBD23, VCRP23, WTST24a, WSV20, WCT+23, WFBB22, WKD+21, YC23, YMM+24, ZG21, ZWY+22, ZFRM20].

E-fields [AMF+20]. **E4** [WS21]. **earth** [ZWL+24a]. **earth-doped** [ZWL+24a]. **ebselen** [YC23]. **EDA** [DGM22, GM22, GKA+23b, SM23]. **EDA-NOCV** [DGM22, GM22, GKA+23b, SM23]. **edge** [CS23]. **Effect** [AD20, DLH+23, GRN20, JC20, ARR22a, BMA+24, CBF+20, DO20, FMK24, FVSS20, JMK+20, KPHV23, KEK23, LK22, LLZ+23, MAM21, MEKH22, dCB23, PRH20, SaATR24, Sts20, SCZ+21, XZW+21]. **effective** [BBC+21a, KKAK23, UB20]. **Effects** [DK23, JFZ+20, KPDB22, KTM+23, MSA22a, SLR+20, SGT+20, JGdC+23, BAM+24, CMG+24, CMO+24, CX21b, FBP+22, GCP22, GAG20, KWYN23, LCLB24, dCB23, MCD22, PCI23, SSSA23, WCY+24, dCVARN20]. **efficiency** [FYIO23, ZWL24b]. **Efficient** [CSGVF+20, LMPT21, MN20, MR21, MKB+21, MT20b, PPV+21, RCC21, XLW+22, AD23, DYGM21, EK20a, KG23, KSRKS21, RD24, TAB+24, ZQ24, ZZG+21]. **efflux** [CGSP24a]. **effort** [POvG21]. **eigenvalues** [KDLP21]. **Eighth** [PSMPB21]. **Eighth-Shell** [PSMPB21]. **elacestrant** [CSP20]. **elastic** [KOD21, LM24, MA23a, MA23b, MMAZ+23, ZLLL22]. **Electric** [PL22, SHM+20, ZG21]. **electride** [Ari24, DSC20]. **electrocatalysts** [AR20]. **electrochemical** [KDLP21, KF24]. **Electrocyclization** [PC21]. **electrode** [DOT22]. **electrolyte** [LEP+21]. **electrolytes** [EG20, HM21]. **Electron** [KZJ22, BJ22, BBC+21a, ĆNF23, EVKL21, EPT21, IN23a, KZJ21, LKT21, LKAT22, LT23, MH22, MAM21, PTP23, PDP+24, RCC+20, RNP20, RTB23, SS20, SPSH20, SMB+23, SSO+20, SZL23, TAC+23, Yos24, ZYZ24, dBCdL20]. **electronegativity** [Vyb23]. **Electronic** [DGSB+20, JX24, SBFSJMLU23, SM22b, SCKH21, TT20, AQIS+24, ABAQ+23, Ari24, AMF+20, BMA+24, BTSB22, CC22, CCPR24, HSG21, IK21, JMV21, KWYN23, KPDB22, Kop22a, LM24, LXP+22, LAM+23,

References

Anisimov:2020:IEC

[AA20] Aleksei A. Anisimov and Ivan V. Ananyev. Interatomic exchange-correlation interaction energy from a measure of quantum theory of atoms in molecules topological bonding: a diatomic case. *Journal of Computational Chemistry*, 41(25): 2213–2222, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alaidi:2020:SMP

[AAe20] Osama Alaidi and Fareed Aboul-ela. Statistical mechanical prediction of ligand perturbation to RNA secondary structure and application to riboswitches. *Journal of Computational Chemistry*, 41(16):1521–1537, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andersson:2021:PCC

[AÅFJ21] Rasmus Andersson, Fabian Årén, Alejandro A. Franco, and Patrik Johansson. CHAMPION: Chalmers hierarchical atomic, molecular, polymeric and ionic analysis toolkit. *Journal of Computational Chemistry*, 42(23):1632–1642, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abbasi:2022:COS

[AAID22] Ali Abbasi, Sepideh Amjad-Iranagh, and Bahram Dabir. CellSys: an open-source tool for building initial structures for biomembranes and drug-delivery systems. *Journal of Computational Chemistry*, 43(5):331–339, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ammar:2021:CGA

[AAL21] Abdallah Ammar, Lorenzo Ugo Ancarani, and Arnaud Leclerc. A complex Gaussian approach to molecular photoionization. *Journal of Computational Chemistry*, 42(32): 2294–2305, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ali:2023:SEM

[ABAQ+23] Malak Azmat Ali, Aboud Ahmed Awadh Bahajjaj, Samah Al-Qaisi, Mika Sillanpää, Afzal Khan, and Xiaoyu Wang. Structural, electronic, magnetic and thermoelectric properties of Tl_2NbX_6 (X = Cl, Br) variant perovskites calculated via density functional theory. *Journal of Computational Chemistry*, 44(23):1875–1883, September 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Avagliano:2022:API

[ABNG22] Davide Avagliano, Matteo Bonfanti, Artur Nenov, and Marco Garavelli. Automatized protocol and interface to simulate QM/MM time-resolved transient absorption at TD-DFT level with COBRAMM. *Journal of Computational Chemistry*, 43 (24):1641–1655, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alcaide:2022:MNM

[ABTM22] Eric Alcaide, Stella Biderman, Amalio Telenti, and M. Cyrus Maher. MP–NeRF: a massively parallel method for accelerating protein structure reconstruction from internal coordinates. *Journal of Computational Chemistry*, 43(1):74–78, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahmadvand:2020:CI

[ABZ20a] Zeinab Ahmadvand, Mehdi Bayat, and Mohammad Ali Zolfigol. Cover image. *Journal of Computational Chemistry*, 41(26):C1, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahmadvand:2020:TPP

[ABZ20b] Zeinab Ahmadvand, Mehdi Bayat, and Mohammad Ali Zolfigol. Toward prediction of the precatalyst activation mechanism through the cross-coupling reactions: Reduction of Pd(II) to Pd(0) in precatalyst of the type Pd-PEPPSI. *Journal of Computational Chemistry*, 41(26):2296–2309, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alzahrani:2020:CAI

[AD20] Khalid A. H. Alzahrani and Robert J. Deeth. A computational analysis of the intrinsic plasticity of five-coordinate Cu(II) complexes and the factors leading to the breakdown of the orbital directing effect in paddlewheel secondary building units. *Journal of Computational Chemistry*, 41(4):340–348, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahirwar:2023:FFM

[AD23] Mini Bharati Ahirwar and Milind M. Deshmukh. Fragments-in-fragments method for efficient and reliable estimates of individual hydrogen bond energies in large molecular clusters. *Journal of Computational Chemistry*, 44(23):1861–1874, September 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Achazi:2024:DMS

[AFR+24a] Andreas J. Achazi, Xhesilda Fataj, Philip Rohland, Martin D. Hager, Ulrich S. Schubert, and Doreen Mollenhauer. Development of a multi-step screening procedure for redox active molecules in organic radical polymer anodes and as redox flow anolytes. *Journal of Computational Chemistry*, 45(14):1112–1129, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Achazi:2024:FC

[AFR+24b] Andreas J. Achazi, Xhesilda Fataj, Philip Rohland, Martin D. Hager, Ulrich S. Schubert, and Doreen Mollenhauer. Front cover. *Journal of Computational Chemistry*, 45(14):C1, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alonso-Gil:2021:PMS

[AG21] Santiago Alonso-Gil. `MonteCarbo`: a software to generate and dock multifunctionalized ring molecules. *Journal of Computational Chemistry*, 42(21):1526–1534, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andoh:2021:AMM

[AiIS+21] Yoshimichi Andoh, Shin ichi Ichikawa, Tatsuya Sakashita, Noriyuki Yoshii, and Susumu Okazaki. Algorithm to minimize MPI communications in the parallelized fast multipole method combined with molecular dynamics calculations. *Journal of Computational Chemistry*, 42(15):1073–1087, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anand:2020:ESI

[AIV20] Neethu Anand, Sai Vamsi Krishna Isukapalli, and Sivaranjana Reddy Vennapusa. Excited-state intramolecular proton transfer driven by conical intersection in hydroxychromones. *Journal of Computational Chemistry*, 41(11):1068–1080, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alipour:2020:ABS

[AK20] Mojtaba Alipour and Kimia Kargar. Anionic behavior and single-molecule crystal in fullerene confinements: a contribution from DFT energy decomposition and cooperativity analyses. *Journal of Computational Chemistry*, 41(21):1912–1920, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahirwar:2024:HBE

[AKGD24] Mini Bharati Ahirwar, Subodh S. Khire, Shridhar R. Gadre, and Milind M. Deshmukh. Hydrogen bond energy estimation (H-BEE) in large molecular clusters: a Python program for quantum chemical investigations. *Journal of Computational Chemistry*, 45(5):274–283, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Akinaga:2020:FSC

[AKN+20] Yoshinobu Akinaga, Koichiro Kato, Tatsuya Nakano, Kaori Fukuzawa, and Yuji Mochizuki. Fragmentation at sp^2 carbon atoms in fragment molecular orbital method. *Journal of Computational Chemistry*, 41(15):1416–1420, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aaroen:2021:PVA

[AKR21] Ola Aarøen, Henrik Kiær, and Enrico Riccardi. PyVisA: Visualization and analysis of path sampling trajectories. *Journal of Computational Chemistry*, 42(6):435–446, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ammar:2020:FCW

[ALA20] Abdallah Ammar, Arnaud Leclerc, and Lorenzo Ugo Ancarani. Fitting continuum wavefunctions with complex Gaussians: Computation of ionization cross sections. *Journal of Computational Chemistry*, 41(27):2365–2377, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arabzadeh:2022:HDL

[ALA+22] Hesam Arabzadeh, Chengwen Liu, Orlando Acevedo, Pengyu Ren, Wei Yang, and Thomas Albrecht-Schönzart. Hydration of divalent lanthanides, Sm^{2+} and Eu^{2+}: a molecular dynamics study with polarizable AMOEBA force field. *Journal of Computational Chemistry*, 43(19):1286–1297, July 15, 2022.

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

Andreadi:2021:PSS

[AME+21] Nikolai Andreadi, Artem Mitrofanov, Artem Eliseev, Petr Matveev, Stepan Kalmykov, and Vladimir Petrov. `PyRad`: A software shell for simulating radiolysis with `Qball` package. *Journal of Computational Chemistry*, 42(13):944–950, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Azizi:2020:NGQ

[AMF+20] Alireza Azizi, Roya Momen, Herbert Früchtl, Tanja van Mourik, Steven R. Kirk, and Samantha Jenkins. Next-generation QTAIM for scoring molecular wires in E-fields for molecular electronic devices. *Journal of Computational Chemistry*, 41(9):913–921, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ali:2022:MSC

[AMM22] Jemal Mohamed Ali, Ahmed Mustefa Mohammed, and Yedilfana Setarge Mekonnen. Mechanistic study on the coupling reaction of CO_2 with propylene oxide catalyzed by $(CH_3)_4PI{\cdot}MgCl_2$. *Journal of Computational Chemistry*, 43 (14):961–971, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CI

[Ano20a] Anonymous. Cover image. *Journal of Computational Chemistry*, 41(25):C1, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVa

[Ano20b] Anonymous. Cover image, volume 41, issue 1. *Journal of Computational Chemistry*, 41(1):C1, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVj

[Ano20c] Anonymous. Cover image, volume 41, issue 10. *Journal of Computational Chemistry*, 41(10):C1, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVk

[Ano20d] Anonymous. Cover image, volume 41, issue 11. *Journal of Computational Chemistry*, 41(11):C1, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVl

[Ano20e] Anonymous. Cover image, volume 41, issue 12. *Journal of Computational Chemistry*, 41(12):C1, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVm

[Ano20f] Anonymous. Cover image, volume 41, issue 12. *Journal of Computational Chemistry*, 41(12):C2, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVo

[Ano20g] Anonymous. Cover image, volume 41, issue 13. *Journal of Computational Chemistry*, 41(13):C1, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVp

[Ano20h] Anonymous. Cover image, volume 41, issue 14. *Journal of Computational Chemistry*, 41(14):C1, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVq

[Ano20i] Anonymous. Cover image, volume 41, issue 15. *Journal of Computational Chemistry*, 41(15):C1, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVr

[Ano20j] Anonymous. Cover image, volume 41, issue 15. *Journal of Computational Chemistry*, 41(15):C4, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVs

[Ano20k] Anonymous. Cover image, volume 41, issue 16. *Journal of Computational Chemistry*, 41(16):C1, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVt

[Ano20l] Anonymous. Cover image, volume 41, issue 17. *Journal of Computational Chemistry*, 41(17):C1, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVu

[Ano20m] Anonymous. Cover image, volume 41, issue 18. *Journal of Computational Chemistry*, 41(18):C1, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVv

[Ano20n] Anonymous. Cover image, volume 41, issue 18. *Journal of Computational Chemistry*, 41(18):C2, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVw

[Ano20o] Anonymous. Cover image, volume 41, issue 19. *Journal of Computational Chemistry*, 41(19):C1, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVb

[Ano20p] Anonymous. Cover image, volume 41, issue 2. *Journal of Computational Chemistry*, 41(2):C1, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVx

[Ano20q] Anonymous. Cover image, volume 41, issue 20. *Journal of Computational Chemistry*, 41(20):C1, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVy

[Ano20r] Anonymous. Cover image, volume 41, issue 21. *Journal of Computational Chemistry*, 41(21):C1, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVz

[Ano20s] Anonymous. Cover image, volume 41, issue 22. *Journal of Computational Chemistry*, 41(22):C1, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVba

[Ano20t] Anonymous. Cover image, volume 41, issue 23. *Journal of Computational Chemistry*, 41(23):C1, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVbb

[Ano20u] Anonymous. Cover image, volume 41, issue 24. *Journal of Computational Chemistry*, 41(24):C1, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVc

[Ano20v] Anonymous. Cover image, volume 41, issue 3. *Journal of Computational Chemistry*, 41(3):C1, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVd

[Ano20w] Anonymous. Cover image, volume 41, issue 4. *Journal of Computational Chemistry*, 41(4):C1, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVe

[Ano20x] Anonymous. Cover image, volume 41, issue 5. *Journal of Computational Chemistry*, 41(5):C1, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVf

[Ano20y] Anonymous. Cover image, volume 41, issue 6. *Journal of Computational Chemistry*, 41(6):C1, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVg

[Ano20z] Anonymous. Cover image, volume 41, issue 7. *Journal of Computational Chemistry*, 41(7):C1, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVh

[Ano20-27] Anonymous. Cover image, volume 41, issue 8. *Journal of Computational Chemistry*, 41(8):C1, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:CIVi

[Ano20-28] Anonymous. Cover image, volume 41, issue 9. *Journal of Computational Chemistry*, 41(9):C1, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIa

[Ano20-29] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(1):1–5, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIb

[Ano20-30] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(2):83–87, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIc

[Ano20-31] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(3):165–170, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IId

[Ano20-32] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(4):273–278, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIe

[Ano20-33] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(5):379–384, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIf

[Ano20-34] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(6):483–488, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIg

[Ano20-35] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(7):605–610, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIh

[Ano20-36] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(8):739–744, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIi

[Ano20-37] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(9):857–861, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIj

[Ano20-38] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(10):971–975, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIk

[Ano20-39] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(11):1059–1063, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIl

[Ano20-40] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(12):1139–1143, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIm

[Ano20-41] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(13):1229–1233, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIn

[Ano20-42] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(14):1325–1329, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIo

[Ano20-43] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(15):1411–1415, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIp

[Ano20-44] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(16):1481–1485, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIq

[Ano20-45] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(17):1571–1575, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIr

[Ano20-46] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(18):1655–1659, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIs

[Ano20-47] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(19):1735–1739, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIt

[Ano20-48] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(20):1799–1803, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIu

[Ano20-49] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(21):1869–1873, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIv

[Ano20-50] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(22):1941–1945, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIw

[Ano20-51] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(23):2017–2021, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIx

[Ano20-52] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(24):2099–2103, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIy

[Ano20-53] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(25):2163–2167, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIz

[Ano20-54] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(26):2223–2227, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIba

[Ano20-55] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(27):2311–2315, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIbb

[Ano20-56] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(28):2383–2387, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIbc

[Ano20-57] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(29):2441–2445, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIbd

[Ano20-58] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(30):2539–2543, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIbe

[Ano20-59] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(31):2605–2609, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2020:IIbf

[Ano20-60] Anonymous. Issue information. *Journal of Computational Chemistry*, 41(32):2679–2683, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIa

[Ano21a] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(1):1–5, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIb

[Ano21b] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(2):67–71, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIc

[Ano21c] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(3):131–135, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIe

[Ano21d] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(4):205–209, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIf

[Ano21e] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(5):265–270, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIg

[Ano21f] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(6):393–397, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIh

[Ano21g] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(7):465–469, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIi

[Ano21h] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(8):523–527, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIj

[Ano21i] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(9):581–585, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIk

[Ano21j] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(10):661–665, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIl

[Ano21k] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(11):735–739, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIm

[Ano21l] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(12):801–805, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIn

[Ano21m] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(13):883–887, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIo

[Ano21n] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(14):951–955, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIp

[Ano21o] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(15):1035–1039, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIq

[Ano21p] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(16):1101–1105, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIr

[Ano21q] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(17):1179–1183, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIs

[Ano21r] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(18):1243–1247, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIt

[Ano21s] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(19):1333–1337, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIu

[Ano21t] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(20):1385–1389, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIv

[Ano21u] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(21):1461–1465, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIw

[Ano21v] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(22):1535–1539, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIx

[Ano21w] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(23):1627–1631, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIy

[Ano21x] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(24):1705–1709, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIz

[Ano21y] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(25):1767–1771, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIba

[Ano21z] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(26):1827–1831, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbb

[Ano21-27] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(27):1915–1919, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbc

[Ano21-28] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(28):1991–1995, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbd

[Ano21-29] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(29):2049–2053, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbe

[Ano21-30] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(30):2131–2135, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbf

[Ano21-31] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(31):2197–2201, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2021:IIbg

[Ano21-32] Anonymous. Issue information. *Journal of Computational Chemistry*, 42(32):2259–2263, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIa

[Ano22a] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(1):1–5, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIb

[Ano22b] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(2):79–83, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIc

[Ano22c] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(3):155–159, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IId

[Ano22d] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(4):225–229, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIe

[Ano22e] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(5):303–307, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIf

[Ano22f] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(6):377–381, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIg

[Ano22g] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(7):435–439, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIh

[Ano22h] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(8):499–503, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIi

[Ano22i] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(9):583–587, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIj

[Ano22j] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(10):655–659, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIk

[Ano22k] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(11):741–745, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIl

[Ano22l] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(12):823–827, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIm

[Ano22m] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(13):889–893, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIn

[Ano22n] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(14):937–941, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIo

[Ano22o] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(15):995–999, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIp

[Ano22p] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(16):1063–1067, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIq

[Ano22q] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(17):1135–1139, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIr

[Ano22r] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(18):1201–1205, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIs

[Ano22s] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(19):1271–1275, July 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIt

[Ano22t] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(20):1329–1333, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIu

[Ano22u] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(21):1389–1393, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIv

[Ano22v] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(22):1459–1463, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIw

[Ano22w] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(23):1525–1529, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIx

[Ano22x] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(24):1609–1613, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIy

[Ano22y] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(25):1675–1679, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIz

[Ano22z] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(26):1759–1763, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIba

[Ano22-27] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(27):1825–1829, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIbb

[Ano22-28] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(28):1887–1891, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIbc

[Ano22-29] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(29):1937–1941, November 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIbd

[Ano22-30] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(30):1997–2000, November 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIbe

[Ano22-31] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(31):2043–2046, December 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2022:IIbf

[Ano22-32] Anonymous. Issue information. *Journal of Computational Chemistry*, 43(32):2099–2102, December 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIa

[Ano23a] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(1):1–4, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIb

[Ano23b] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(2):61–64, January 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIc

[Ano23c] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(3):117–128, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IId

[Ano23d] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(4):489–494, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIe

[Ano23e] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(5):657–661, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIf

[Ano23f] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(6):727–731, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIg

[Ano23g] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(7):801–805, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIh

[Ano23h] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(8):869–873, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIi

[Ano23i] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(9):949–953, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIj

[Ano23j] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(10):1011–1015, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIk

[Ano23k] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(11):1089–1093, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIl

[Ano23l] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(12):1159–1163, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIm

[Ano23m] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(13):1231–1235, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIn

[Ano23n] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(14):1329–1333, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIo

[Ano23o] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(15):1405–1409, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIp

[Ano23p] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(16):1465–1469, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIq

[Ano23q] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(17):1531–1535, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIr

[Ano23r] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(18):1599–1603, July 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIs

[Ano23s] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(19):1653–1657, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIt

[Ano23t] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(20):1715–1718, July 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIu

[Ano23u] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(21):1767–1770, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIv

[Ano23v] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(22):1803–1806, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIw

[Ano23w] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(23):1857–1860, September 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIx

[Ano23x] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(24):1913–1916, September 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIy

[Ano23y] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(25):1971–1975, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIz

[Ano23z] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(26):2037–2041, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIba

[Ano23-27] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(27):2103–2107, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIbb

[Ano23-28] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(28):2161–2165, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIbc

[Ano23-29] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(29):2241–2245, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIbd

[Ano23-30] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(30):2303–2307, November 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIbe

[Ano23-31] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(31):2369–2373, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2023:IIbf

[Ano23-32] Anonymous. Issue information. *Journal of Computational Chemistry*, 44(32):2437–2441, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:CTE

[Ano24a] Anonymous. Correction to "Terminal end-on coordination of dinitrogen vs. isoelectronic CO: a comparison using the charge displacement analysis". *Journal of Computational Chemistry*, 45(4):230–232, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [SK23].

Anonymous:2024:IIa

[Ano24b] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(1):1–5, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIb

[Ano24c] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(2):65–69, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIc

[Ano24d] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(3):135–139, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IId

[Ano24e] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(4):193–196, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIe

[Ano24f] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(5):233–237, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIf

[Ano24g] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(6):301–305, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIg

[Ano24h] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(7):363–367, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIh

[Ano24i] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(8):431–435, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIi

[Ano24j] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(9):507–511, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIj

[Ano24k] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(10):589–594, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIk

[Ano24l] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(11):695–700, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIl

[Ano24m] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(12):821–826, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIm

[Ano24n] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(13):931–936, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIn

[Ano24o] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(14):1061–1066, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIo

[Ano24p] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(15):1187–1192, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIp

[Ano24q] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(16):1317–1321, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIq

[Ano24r] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(17):1429–1433, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anonymous:2024:IIr

[Ano24s] Anonymous. Issue information. *Journal of Computational Chemistry*, 45(18):1525–1529, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aarabi:2024:FHR

[APP24] Mahdi Aarabi, Ankit Pandey, and Bill Poirier. "On-the-fly": How to reliably and automatically characterize and construct potential energy surfaces. *Journal of Computational Chemistry*, 45(15):1261–1278, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arrue:2021:SCB

[APR21] Lily Arrué and Ricardo Pino-Rios. On the stability and chemical bond of noble gas halide cations NgX^+ (Ng = He–Rn; X = F–I). *Journal of Computational Chemistry*, 42(2):124–129, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahn:2020:PWA

[APS20] Dae-Hwan Ahn, Chiyoung Park, and Jong-Won Song. Predicting whether aromatic molecules would prefer to enter a carbon nanotube: a density functional theory study. *Journal of Computational Chemistry*, 41(13):1261–1270, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Al-Qaisi:2024:OET

[AQIS+24] Samah Al-Qaisi, Nazia Iram, Saidi Samah, Afaf Khadr Alqorashi, A. I. Aljameel, Tahani A. Alrebdi, Zeesham Abbas, S. Bouzgarrou, Md. Ferdous Rahman, and Ajay Singh Verma. Opto-electronic and thermophysical characteristics of A_2TlAgF_6 (a = Rb, Cs) for green technology applications. *Journal of Computational Chemistry*, 45(18):1576–1586, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Al-Qaisi:2023:TIL

[AQMM+23] Samah Al-Qaisi, Abdelazim M. Mebed, Muhammad Mushtaq, D. P. Rai, Tahani A. Alrebdi, Rais Ahmad Sheikh, Habib Rached, R. Ahmed, Muhammad Faizan, S. Bouzgarrou, and Muhammad Anjum Javed. A theoretical investigation of the lead-free double perovskites halides Rb_2XCl_6 (X = Se, Ti) for optoelectronic and thermoelectric applications. *Journal of Computational Chemistry*, 44(19):1690–1703, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Al-Qaisi:2023:SMO

[AQRA+23] Samah Al-Qaisi, Habib Rached, Tahani A. Alrebdi, S. Bouzgarrou, Debidatta Behera, Sanat Kumar Mukherjee, Mohamed Khuili, Mohamed Adam, Ajay Singh Verma, and Mohammed Ezzeldien. Study of mechanical, optical, and thermoelectric characteristics of Ba_2XMoO_6 (X = Zn, Cd) double perovskite for energy harvesting. *Journal of Computational Chemistry*, 44(32):2442–2452, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ananthaneni:2020:CST

[AR20] Sahithi Ananthaneni and Rees B. Rankin. Computational screening of transition metal/p-block hybrid electrocatalysts for CO_2 reduction. *Journal of Computational Chemistry*, 41 (14):1384–1394, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andolpho:2024:PBD

[AR24] Gustavo A. Andolpho and Teodorico C. Ramalho. Pnictogen bond-driven control of the molecular interaction between organophosphorus and acetylcholinesterase enzyme. *Journal* *of Computational Chemistry*, 45(15):1303–1315, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Abdullayev:2022:CMS

[ARA22] Yusif Abdullayev, Ramil Rzayev, and Jochen Autschbach. Computational mechanistic studies on persulfate assisted p-phenylenediamine polymerization. *Journal of Computational Chemistry*, 43(19):1313–1319, July 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ariyarathna:2024:GEE

[Ari24] Isuru R. Ariyarathna. Ground and excited electronic structures of electride and alkalide units: The cases of Metal-Tren, -Azacryptand, and -TriPip222 complexes. *Journal of Computational Chemistry*, 45(10):655–662, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Afonin:2022:GTC

[ARR22a] Andrei V. Afonin and Danuta Rusinska-Roszak. Guide to tuning the chalcone molecular properties based on the push-pull effect energy scale created via the molecular tailoring approach. *Journal of Computational Chemistry*, 43(9):631–643, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Afonin:2022:MTA

[ARR22b] Andrei V. Afonin and Danuta Rusinska-Roszak. Molecular tailoring approach as tool for revealing resonance-assisted hydrogen bond: Case study of *Z*-pyrrolylenones with the N–H$\cdots$O$=$C intramolecular hydrogen bond. *Journal of Computational Chemistry*, 43(23):1596–1607, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anjali:2020:AEP

[AS20] Bai A. Anjali and Cherumuttathu H. Suresh. Absorption and emission properties of 5-phenyl tris(8-hydroxyquinolinato) M(III) complexes (M = Al, Ga, In) and correlations with molecular electrostatic potential. *Journal of Computational Chemistry*, 41(16):1497–1508, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ahn:2021:ALR

[AS21] Dae-Hwan Ahn and Jong-Won Song. Assessment of long-range corrected density functional theory on the absorption and vibrationally resolved fluorescence spectrum of carbon nanobelts. *Journal of Computational Chemistry*, 42(7):505–515, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anila:2023:FMS

[AS23] Sebastian Anila and Cherumuttathu H. Suresh. Fulleride-metal η^5 sandwich and multi-decker sandwich complexes: a DFT prediction. *Journal of Computational Chemistry*, 44(3): 199–208, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alberto:2020:ISP

[ASL+20] Marta Erminia Alberto, Bruna Clara De Simone, Simona Liuzzi, Tiziana Marino, Nino Russo, and Marirosa Toscano. Iodine substituted phosphorus corrole complexes as possible photosensitizers in photodynamic therapy: Insights from theory. *Journal of Computational Chemistry*, 41(14):1395–1401, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Alag:2024:IIE

[AST24] Ahmed Shaalan Alag, Péter G. Szalay, and Attila Tajti. Ab initio investigation of excited state charge transfer pathways in differently capped bithiophene cages. *Journal of Computational Chemistry*, 45(14):1078–1086, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Aquino:2020:FON

[ASW20] Fredy W. Aquino, Ravindra Shinde, and Bryan M. Wong. Fractional occupation numbers and self-interaction correction-scaling methods with the Fermi–Löwdin orbital self-interaction correction approach. *Journal of Computational Chemistry*, 41 (12):1200–1208, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Afonin:2020:QDR

[AV20] Andrei V. Afonin and Alexander V. Vashchenko. Quantitative decomposition of resonance-assisted hydrogen bond energy in

β-diketones into resonance and hydrogen bonding (π- and σ-) components using molecular tailoring and function-based approaches. *Journal of Computational Chemistry*, 41(13):1285–1298, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arroyuelo:2021:EQP

[AVM21] Agustina Arroyuelo, Jorge A. Vila, and Osvaldo A. Martin. Exploring the quality of protein structural models from a Bayesian perspective. *Journal of Computational Chemistry*, 42(21):1466–1474, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Awoonor-Williams:2020:QCM

[AWID+20] Ernest Awoonor-Williams, William C. Isley III, Stephen G. Dale, Erin R. Johnson, Haibo Yu, Axel D. Becke, Benoît Roux, and Christopher N. Rowley. Quantum chemical methods for modeling covalent modification of biological thiols. *Journal of Computational Chemistry*, 41(5):427–438, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Anders:2023:CBH

[AWK+23] Jennifer Anders, Henrik Wiedenhaupt, Florian Kreuter, Ralf Tonner-Zech, and Beate Paulus. Chemical bonding of HF, HCl, and H_2O onto YF_3 surfaces: Quantification by first principles. *Journal of Computational Chemistry*, 44(25):1986–1997, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andoh:2020:EFM

[AYO20] Yoshimichi Andoh, Noriyuki Yoshii, and Susumu Okazaki. Extension of the fast multipole method for the rectangular cells with an anisotropic partition tree structure. *Journal of Computational Chemistry*, 41(14):1353–1367, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Andreadi:2022:TPE

[AZKM22] Nikolai Andreadi, Dmitry Zankov, Kirill Karpov, and Artem Mitrofanov. Tree Parzen estimator for global geometry optimization: a benchmark and database of experimental gas-phase structures of organic molecules. *Journal of Computa-*

tional Chemistry, 43(21):1434–1441, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bae:2022:TDD

[BA22] Gyun-Tack Bae and Christine M. Aikens. Time-dependent density functional theory study of the optical properties of tetrahedral aluminum nanoparticles. *Journal of Computational Chemistry*, 43(15):1033–1041, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barrera:2024:DRG

[BA24] Yoshio Barrera and James S. M. Anderson. Does the radical GPRI strongly depend on the population scheme? A comparative study to predict radical attack on unsaturated molecules with the radical general-purpose reactivity indicator. *Journal of Computational Chemistry*, 45(14):1152–1159, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beu:2020:MFF

[BAC20] Titus Adrian Beu, Andrada-Elena Ailenei, and Razvan-Ioan Costinas. Martini force field for protonated polyethyleneimine. *Journal of Computational Chemistry*, 41(4):349–361, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:2020:CCH

[Bal20a] Krishnan Balasubramanian. Computations of colorings 7D-hypercube's hyperplanes for all irreducible representations. *Journal of Computational Chemistry*, 41(7):653–686, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balasubramanian:2020:NWO

[Bal20b] Krishnan Balasubramanian. Nonrigid water octamer: Computations with the 8-cube. *Journal of Computational Chemistry*, 41(29):2469–2484, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boutiddar:2024:IMC

[BAM+24] Rachid Boutiddar, Khalid Abbiche, Moulay Driss Mellaoui, Abdallah Imjjad, Mustapha Alahiane, Youssef Ait Albrimi, Khadija Marakchi, Muneerah Mogren Al-Mogren, Abdellatif El Hammadi, and Majdi Hochlaf. Insights into the mechanism of $[3+2]$ cycloaddition reactions between N-benzyl fluoro nitrone and maleimides, its selectivity and solvent effects. *Journal of Computational Chemistry*, 45(5):284–299, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Banavali:2020:MCM

[Ban20] Nilesh K. Banavali. The mechanism of cholesterol modification of hedgehog ligand. *Journal of Computational Chemistry*, 41 (6):520–527, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bekker:2020:ESC

[BAO$^+$20] Gert-Jan Bekker, Mitsugu Araki, Kanji Oshima, Yasushi Okuno, and Narutoshi Kamiya. Exhaustive search of the configurational space of heat-shock protein 90 with its inhibitor by multicanonical molecular dynamics based dynamic docking. *Journal of Computational Chemistry*, 41(17):1606–1615, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brodney:2023:IDE

[BBB$^+$23] Marian D. Brodney, Gregory Bakken, Christopher R. Butler, Jacquelyn Klug-McLeod, Robert Owen, and Shao-Tien Sng. Integrated design environment: a multi-use platform for design idea capture, evaluation, and tracking in medicinal chemistry. *Journal of Computational Chemistry*, 44(6): 788–800, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Briccolani-Bandini:2023:CVS

[BBBP$^+$23] Lorenzo Briccolani-Bandini, Eric Brémond, Marco Pagliai, Gianni Cardini, Ilaria Ciofini, and Carlo Adamo. Concerted versus stepwise proton transfer reactions in the [2, 2'-bipyridyl]-3-3'-diol molecule: a static and dynamic ab-initio investigation. *Journal of Computational Chemistry*, 44(30):2308–2318, November 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Banik:2020:QMS

[BBC20] Sindrila Dutta Banik, Arindam Bankura, and Amalendu Chandra. A QM/MM simulation study of transamination reaction at the active site of aspartate aminotransferase: Free energy landscape and proton transfer pathways. *Journal of Computational Chemistry*, 41(32):2684–2694, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Blasiak:2021:IEO

[BBC+21a] Bartosz Błasiak, Joanna D. Bednarska, Marta Chołuj, Robert W. Góra, and Wojciech Bartkowiak. Ab initio effective one-electron potential operators: Applications for charge-transfer energy in effective fragment potentials. *Journal of Computational Chemistry*, 42(6):398–411, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Blasiak:2021:CI

[BBC+21b] Bartosz Błasiak, Joanna D. Bednarska, Marta Chołuj, Robert W. Góra, and Wojciech Bartkowiak. Cover image. *Journal of Computational Chemistry*, 42(6):C1, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boruah:2020:PRS

[BBK20] Abhijit Boruah, Manash Protim Borpuzari, and Rahul Kar. Performance of range separated density functional in solvent continuum: Tuning long-range Hartree–Fock exchange for improved orbital energies. *Journal of Computational Chemistry*, 41(4):295–304, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brabec:2021:MPQ

[BBK+21] Jiri Brabec, Jan Brandejs, Karol Kowalski, Sotiris Xantheas, Örs Legeza, and Libor Veis. Massively parallel quantum chemical density matrix renormalization group method. *Journal of Computational Chemistry*, 42(8):534–544, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Boziki:2022:TPU

[BBL+22] Ariadni Boziki, Pablo Baudin, Elisa Liberatore, Negar Ashari Astani, and Ursula Rothlisberger. A theoretical perspective of the ultrafast transient absorption dynamics of $CsPbBr_3$. *Journal of Computational Chemistry*, 43(8):577–582, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barletta:2022:ACC

[BBSFA22] German P. Barletta, Matias Barletta, Tadeo E. Saldaño, and Sebastian Fernandez-Alberti. Analysis of changes of cavity volumes in predefined directions of protein motions and cavity flexibility. *Journal of Computational Chemistry*, 43(6):391–401, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bai:2021:FRD

[BBY+21] Yuwen Bai, Bayaer Buren, Zijiang Yang, Boyi Zhou, and Maodu Chen. Feshbach resonances in D + HD ($v = 1, j = 0$) reaction at low collision energies. *Journal of Computational Chemistry*, 42(32):2334–2340, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bruce-Chwatt:2022:MMR

[BCN22] Tomás Bruce-Chwatt and Kevin J. Naidoo. Molecular mechanisms from reaction coordinate graph enabled multidimensional free energies illustrated on water dimer hydrogen bonding. *Journal of Computational Chemistry*, 43(26):1802–1813, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borah:2022:SZG

[BD22] Ritam R. Borah and Rinu P. Deka. Stabilization of Zn group dimers: a theoretical study. *Journal of Computational Chemistry*, 43(25):1719–1724, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bates:2021:CIB

[BdLC21] Thomas G. Bates, Jurgens H. de Lange, and Ignacy Cukrowski. The CH$\cdots$HC interaction in biphenyl is a delocalized, molecular-wide and entirely non-classical interaction: Results from FALDI analysis. *Journal of Computa-*

tional Chemistry, 42(10):706–718, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bodo:2024:CBU

[BEKM24] Filippo Bodo, Alessandro Erba, Elfi Kraka, and Renaldo T. Moura, Jr. Chemical bonding in uranium-based materials: a local vibrational mode case study of Cs UO Cl and UCl crystals. *Journal of Computational Chemistry*, 45(14):1130–1142, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benassi:2022:IDF

[Ben22] Enrico Benassi. An inexpensive density functional theory-based protocol to predict accurate ^{19}F-NMR chemical shifts. *Journal of Computational Chemistry*, 43(3):170–183, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brankin:2022:PAR

[BF22] Alice E. Brankin and Philip W. Fowler. Predicting antibiotic resistance in complex protein targets using alchemical free energy methods. *Journal of Computational Chemistry*, 43(26): 1771–1782, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baez-Grez:2024:ASB

[BGPR24] Rodrigo Báez-Grez and Ricardo Pino-Rios. On the aromaticity and stability of benzynes in the ground and lowest-lying triplet excited states. *Journal of Computational Chemistry*, 45(1):6–12, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borocci:2020:CHN

[BGS+20] Stefano Borocci, Felice Grandinetti, Nico Sanna, Paola Antoniotti, and Francesca Nunzi. Complexes of helium with neutral molecules: Progress toward a quantitative scale of bonding character. *Journal of Computational Chemistry*, 41(10):1000–1011, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

BenSaid:2021:ENS

[BHR+21] Ridha Ben Said, Riadh Hanachi, Seyfeddine Rahali, Mohammed A. M. Alkhalifah, Faisal Alresheedi, Bahoueddine

Tangour, and Majdi Hochlaf. Evaluation of a new series of pyrazole derivatives as a potent epidermal growth factor receptor inhibitory activity: QSAR modeling using quantum-chemical descriptors. *Journal of Computational Chemistry*, 42(32):2306–2320, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bertolini:2022:VEC

[BJ22] Samuel Bertolini and Timo Jacob. Valence energy correction for electron reactive force field. *Journal of Computational Chemistry*, 43(12):870–878, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baek:2022:DSF

[BK22] Kristoffer T. Bæk and Kasper P. Kepp. Data set and fitting dependencies when estimating protein mutant stability: Toward simple, balanced, and interpretable models. *Journal of Computational Chemistry*, 43(8):504–518, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Buchhorn:2024:APF

[BK24] Moritz Buchhorn and Vera Krewald. AOMadillo: a program for fitting angular overlap model parameters. *Journal of Computational Chemistry*, 45(2):122–134, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bankiewicz:2021:TML

[BKM21] Barbara Bankiewicz, Stephan Kupfer, and Piotr Matczak. Tuning the metal-ligand bond in the σ-complexes of stannylenes and azabenzenes. *Journal of Computational Chemistry*, 42(29):2103–2115, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bayati:2020:HPT

[BLB20] Mahsa Bayati, Miriam Leeser, and Jaydeep P. Bardhan. High-performance transformation of protein structure representation from internal to Cartesian coordinates. *Journal of Computational Chemistry*, 41(24):2104–2114, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bader:2020:VCM

[BLP20] Frederik Bader, Tilen Lindic, and Beate Paulus. A validation of cluster modeling in the description of matrix isolation spectroscopy. *Journal of Computational Chemistry*, 41(8):751–758, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balakrishnan:2024:TIS

[BMA+24] Jothi Balakrishnan, Pavithrakumar Muthukumar, David Stephen Arputharaj, Pitchumani Violet Mary Christopher, Selvaraju Karuppannan, and Senthilkumar Kittusamy. Theoretical investigations of the substituent effect on the opto-electronic properties of the linearly fused napthadithiophene-based molecules. *Journal of Computational Chemistry*, 45(12):915–929, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brown:2021:MCP

[BMT+21] Kristopher Brown, Yasheng Maimaiti, Kai Trepte, Thomas Bligaard, and Johannes Voss. MCML: Combining physical constraints with experimental data for a multi-purpose meta-generalized gradient approximation. *Journal of Computational Chemistry*, 42(28):2004–2013, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Blanc:2023:PLM

[BMT23] Ambre Blanc, Antonio Monari, and Jean Christophe Tremblay. A posteriori localization of many-body excited states through simultaneous diagonalization. *Journal of Computational Chemistry*, 44(2):105–116, January 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [WFLZ23].

Bremond:2021:ACI

[BOPJ+21a] Éric Brémond, Alistar Ottochian, Ángel José Pérez-Jiménez, Ilaria Ciofini, Giovanni Scalmani, Michael J. Frisch, Juan Carlos Sancho-García, and Carlo Adamo. Assessing challenging intra- and inter-molecular charge-transfer excitations energies with double-hybrid density functionals. *Journal of Computational Chemistry*, 42(14):970–981, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bremond:2021:CI

[BOPJ+21b] Éric Brémond, Alistar Ottochian, Ángel José Pérez-Jiménez, Ilaria Ciofini, Giovanni Scalmani, Michael J. Frisch, Juan Carlos Sancho-García, and Carlo Adamo. Cover image. *Journal of Computational Chemistry*, 42(14), May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Burn:2022:PCA

[BP22] Matthew J. Burn and Paul L. A. Popelier. Producing chemically accurate atomic Gaussian process regression models by active learning for molecular simulation. *Journal of Computational Chemistry*, 43(31):2084–2098, December 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bedford:2021:NPI

[BPDG21] John T. Bedford, Jennifer Poutsma, Norou Diawara, and Lesley H. Greene. The nature of persistent interactions in two model β-grasp proteins reveals the advantage of symmetry in stability. *Journal of Computational Chemistry*, 42(9):600–607, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bai:2022:SGS

[BPL+22] Fangyun Bai, Kin Ming Puk, Jin Liu, Hongyu Zhou, Peng Tao, Wenyong Zhou, and Shouyi Wang. Sparse group selection and analysis of function-related residue for protein-state recognition. *Journal of Computational Chemistry*, 43(20):1342–1354, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bajpai:2023:IIC

[BPT+23] Shitanshu Bajpai, Brian K. Petkov, Muchen Tong, Charlles R. A. Abreu, Nisanth N. Nair, and Mark E. Tuckerman. An interoperable implementation of collective-variable based enhanced sampling methods in extended phase space within the `OpenMM` package. *Journal of Computational Chemistry*, 44(28): 2166–2183, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bode:2023:MDS

[BR23] Jan Bode and Gabriele Raabe. Molecular dynamics studies of the solubility behavior of carbon dioxide (CO_2), difluoromethane (r-32), 1-chloro-3,3,3-trifluoropropene (R-1233zd(E)) and 2,3,3,3-tetrafluoro-1-propene (r-1234yf) in pentaerythritol tetra(2-ethylhexanoate) (PEB8), pentaerythritol tetrabutyrate (PEC4) and pentaerythritol tetraoctanoate (PEC8). *Journal of Computational Chemistry*, 44 (29):2274–2283, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beck:2021:UIH

[BRNB21] Michael Edmund Beck, Christoph Riplinger, Frank Neese, and Giovanni Bistoni. Unraveling individual host-guest interactions in molecular recognition from first principles quantum mechanics: Insights into the nature of nicotinic acetylcholine receptor agonist binding. *Journal of Computational Chemistry*, 42(5):293–302, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brzeski:2022:ITB

[Brz22] Jakub Brzeski. The influence of tetrel bonds on the acidities of group 14 tetrafluoride–inorganic acid complexes. *Journal of Computational Chemistry*, 43(9):611–618, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brzeski:2023:ABL

[Brz23] Jakub Brzeski. Aluminabenzene-based Lewis superacids and weakly coordinating anions. *Journal of Computational Chemistry*, 44(15):1454–1463, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bandyopadhyay:2023:MCG

[BS23] Prasanta Bandyopadhyay and Mainak Sadhukhan. Modeling coarse-grained van der Waals interactions using dipole-coupled anisotropic quantum Drude oscillators. *Journal of Computational Chemistry*, 44(12):1164–1173, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bosy:2024:CFB

[BSB+24] Michał Bosy, Matthew W. Scroggs, Timo Betcke, Erik Burman, and Christopher D. Cooper. Coupling finite and boundary element methods to solve the Poisson–Boltzmann equation for electrostatics in molecular solvation. *Journal of Computational Chemistry*, 45(11):787–797, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bozkaya:2020:SAC

[BSF20] Ugur Bozkaya, Emine Soydas, and Bahar Filiz. State-of-the-art computations of dipole moments using analytic gradients of high-level density-fitted coupled-cluster methods with focal-point approximations. *Journal of Computational Chemistry*, 41(8):769–779, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Botello-Smith:2020:IPP

[BSL20] Wesley M. Botello-Smith and Yun Luo. Investigating protein-protein allosteric network using current-flow scheme. *Journal of Computational Chemistry*, 41(6):552–560, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benchehaima:2022:NOP

[BSR22] Fatima-Zohra Benchehaima, Michael Springborg, and Majda Sekkal Rahal. Nonlinear optical properties DFT calculations of polyacethylene and copolymers models substituted with aldimines chromophores as side chains. *Journal of Computational Chemistry*, 43(25):1701–1718, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Barcza:2022:CAI

[BSS+22] Bónis Barcza, Ádám B. Szirmai, Katalin J. Szántó, Attila Tajti, and Péter G. Szalay. Comparison of approximate intermolecular potentials for ab initio fragment calculations on medium sized N-heterocycles. *Journal of Computational Chemistry*, 43(16):1079–1093, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Balius:2024:DIH

[BTC24] Trent E. Balius, Y. Stanley Tan, and Mayukh Chakrabarti. DOCK 6: Incorporating hierarchical traversal through precomputed ligand conformations to enable large-scale docking. *Journal of Computational Chemistry*, 45(1):47–63, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bouchouireb:2024:DCC

[BTL24] Zakaria Bouchouireb, Steeve H. Thany, and Jean-Yves Le Questel. Development of CHARMM compatible force field parameters and molecular dynamics simulations for the pesticide flupyradifurone. *Journal of Computational Chemistry*, 45(7):377–391, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Benedek:2022:SCC

[BTSB22] Zsolt Benedek, Paula Timár, Tibor Szilvási, and Gergely Barcza. Sensitivity of coupled cluster electronic properties on the reference determinant: Can Kohn–Sham orbitals be more beneficial than Hartree–Fock orbitals? *Journal of Computational Chemistry*, 43(32):2103–2120, December 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baba:2022:CI

[BUNO22a] Hiromi Baba, Ryo Urano, Tetsuro Nagai, and Susumu Okazaki. Cover image. *Journal of Computational Chemistry*, 43(28):i, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Baba:2022:PSD

[BUNO22b] Hiromi Baba, Ryo Urano, Tetsuro Nagai, and Susumu Okazaki. Prediction of self-diffusion coefficients of chemically diverse pure liquids by all-atom molecular dynamics simulations. *Journal of Computational Chemistry*, 43(28):1892–1900, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Byun:2023:CRK

[BVC+23] Jinyoung Byun, Srivithya Vellampatti, Prathit Chatterjee, Sun Ha Hwang, Byoung Choul Kim, and Juyong Lee. Characterization of the role of kunitz-type protease inhibitor domain in dimerization of amyloid precursor protein. *Journal of Computational Chemistry*, 44(15):1437–1445, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Beal:2023:PAG

[BVGB23] Roiney Beal, Danillo Valverde, Paulo F. B. Gonçalvez, and Antonio Carlos Borin. Photophysics of ^{tz}Adenine and ^{tz}Guanine fluorescent nucleobases embedded into DNA and RNA. *Journal of Computational Chemistry*, 44(29):2246–2255, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Badorrek:2022:CSN

[BW22a] Jan Badorrek and Michael Walter. Computational study on noncovalent interactions between (n, n) single-walled carbon nanotubes and simple lignin model-compounds. *Journal of Computational Chemistry*, 43(5):340–348, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Brzyska:2022:STS

[BW22b] Agnieszka Brzyska and Krzysztof Wolinski. Search for transition states with external forces. *Journal of Computational Chemistry*, 43(9):598–610, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bhattarai:2020:GPC

[BWM20] Apurba Bhattarai, Jinan Wang, and Yinglong Miao. G-protein-coupled receptor-membrane interactions depend on the receptor activation state. *Journal of Computational Chemistry*, 41(5):460–471, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Badalov:2020:PPG

[BWS20] Sabuhi V. Badalov, René Wilhelm, and Wolf G. Schmidt. Photocatalytic properties of graphene-supported titania clusters from density-functional theory. *Journal of Computational Chemistry*, 41(21):1921–1930, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Bai:2024:MSN

[BXY+24] Yuna Bai, Anmei Xian, Xing Yang, Ming Zhou, Xuefei Zhao, and Lili Zhao. Mechanistic study of the Ni-catalyzed hydroalkylation of 1,3-dienes: The origins of regio- and enantioselectivities and a further rational design. *Journal of Computational Chemistry*, 45(10):610–621, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Curtolo:2022:MPT

[CA22] Felipe Curtolo and Guilherme M. Arantes. Molecular properties and tautomeric equilibria of isolated flavins. *Journal of Computational Chemistry*, 43(23):1561–1572, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ciancaleoni:2020:DOH

[CB20] Gianluca Ciancaleoni and Leonardo Belpassi. Disentanglement of orthogonal hydrogen and halogen bonds via natural orbital for chemical valence: a charge displacement analysis. *Journal of Computational Chemistry*, 41(12):1185–1193, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crowet:2021:LDD

[CBB+21] Jean-Marc Crowet, Sébastien Buchoux, Nicolas Belloy, Catherine Sarazin, Laurence Lins, and Manuel Dauchez. LIMONADA: A database dedicated to the simulation of biological membranes. *Journal of Computational Chemistry*, 42(14):1028–1033, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chenouf:2020:EEC

[CBF+20] Jamal Chenouf, Mourad Boutahir, Brahim Fakrach, Abdelhai Rahmani, Hassane Chadli, Patrick Hermet, Jose Mejía-López, and Abdelali Rahmani. Encapsulation effect of π-conjugated quaterthiophene on the radial breathing and tangential modes of semiconducting and metallic single-walled carbon nanotubes. *Journal of Computational Chemistry*, 41 (28):2420–2428, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chuntakaruk:2024:MLG

[CBK+24] Hathaichanok Chuntakaruk, Kajjana Boonpalit, Jiramet Kinchagawat, Fahsai Nakarin, Tanatorn Khotavivattana, Chanat Aonbangkhen, Yasuteru Shigeta, Kowit Hengphasatporn, Sarana Nutanong, Thanyada Rungrotmongkol, and Supot Hannongbua. Machine learning-guided design of potent darunavir analogs targeting HIV-1 proteases: a computational approach for antiretroviral drug discovery. *Journal of Computational Chemistry*, 45(13):953–968, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cammi:2022:SDE

[CC22] Roberto Cammi and Bo Chen. The second derivative of the electronic energy with respect to the compression scaling factor in the XP-PCM model: Theory and applications to compression response functions of atoms. *Journal of Computational Chemistry*, 43(17):1176–1185, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cho:2023:CIE

[CCHS23] Myung Keun Cho, Song-Ho Chong, Sihyun Ham, and Seokmin Shin. Comparing the influence of explicit and implicit solvation models on site-specific thermodynamic stability of proteins. *Journal of Computational Chemistry*, 44(25):1976–1985, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Crisci:2024:TUT

[CCPR24] Luigi Crisci, Federico Coppola, Alessio Petrone, and Nadia Rega. Tuning ultrafast time-evolution of photo-induced charge-transfer states: a real-time electronic dynamics study in substituted indenotetracene derivatives. *Journal of Computational Chemistry*, 45(4):210–221, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Capar:2023:WOL

[CCZ23] M. Ilk Capar, A. Cetin, and A. V. Zakharov. Water/organic liquid interface properties with amine, carboxyl, thiol, and methyl terminal groups as seen from MD simulations. *Journal of Computational Chemistry*, 44(31):2404–2413, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cheng:2020:ADM

[CD20] Qianyi Cheng and Nathan J. DeYonker. Acylation and deacylation mechanism and kinetics of penicillin G reaction with *Streptomyces* R61 DD-peptidase. *Journal of Computational Chemistry*, 41(18):1685–1697, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2021:MSM

[CDCT21] Wallace K. B. Chan, Debarati DasGupta, Heather A. Carlson, and John R. Traynor. Mixed-solvent molecular dynamics simulation-based discovery of a putative allosteric site on regulator of G protein signaling 4. *Journal of Computational Chemistry*, 42(30):2170–2180, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casier:2021:HLG

[CdSB+21] Bastien Casier, Mauricio Chagas da Silva, Michael Badawi, Fabien Pascale, Tomás Bucko, Sébastien Lebègue, and Dario Rocca. Hybrid localized graph kernel for machine learning energy-related properties of molecules and solids. *Journal of Computational Chemistry*, 42(20):1390–1401, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cervinka:2022:TQH

[Cer22] Ctirad Cervinka. Tuning the quasi-harmonic treatment of crystalline ionic liquids within the density functional theory. *Journal of Computational Chemistry*, 43(7):448–456, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campos-Fernandez:2022:IND

[CFOMCB+22] Linda Campos-Fernández, Rocío Ortiz-Muñiz, Edith Cortés-Barberena, Sergio Mares-Sámano, Ramón Garduño-Juárez, and Catalina Soriano-Correa. Imidazole and nitroimidazole derivatives as NADH-fumarate reductase inhibitors: Density functional theory studies, homology modeling, and molecular docking. *Journal of Computational Chemistry*, 43(23):1573–1595, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Campetella:2020:FEE

[CG20] Marco Campetella and Juan Sanz García. Following the evolution of excited states along photochemical reaction pathways. *Journal of Computational Chemistry*, 41(12):1156–1164, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carreon-Gonzalez:2022:CRD

[CGMRVBAI22] Mirzam Carreon-Gonzalez, Leonardo Muñoz-Rugeles, Annik Vivier-Bunge, and Juan Raul Alvarez-Idaboy. Chemical repair of damaged leucine and tryptophane by thiophenols at close to diffusion-controlled rates: Mechanisms and kinetics. *Journal of Computational Chemistry*, 43(8):556–567, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chauhan:2024:DTI

[CGSP24a] Shweta Singh Chauhan, Anshika Gupta, Aashna Srivastava, and Ramakrishnan Parthasarathi. Discovering targeted inhibitors for *Escherichia coli* efflux pump fusion proteins using computational and structure-guided approaches. *Journal of Computational Chemistry*, 45(1):13–24, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chauhan:2024:FC

[CGSP24b] Shweta Singh Chauhan, Anshika Gupta, Aashna Srivastava, and Ramakrishnan Parthasarathi. Front cover. *Journal of Computational Chemistry*, 45(1):C1, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chong:2023:ECA

[CH23] Song-Ho Chong and Sihyun Ham. Evolutionary conservation of amino acids contributing to the protein folding transition state. *Journal of Computational Chemistry*, 44(9):1002–1009, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2024:LFA

[Cha24] Bun Chan. Limiting factors in the accuracy of DFT calculation for redox potentials. *Journal of Computational Chem-*

istry, 45(14):1177–1186, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2023:PPM

[Che23] Guang Chen. 4polyGraft 1.0: a program for molecular structure and topology generation of polymer-grafted hybrid nanostructures. *Journal of Computational Chemistry*, 44(28):2230–2239, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2021:PIL

[CHVF21] Yixiang Cao, Mathew D. Halls, Tati Reddy Vadicherla, and Richard A. Friesner. Pseudospectral implementations of long-range corrected density functional theory. *Journal of Computational Chemistry*, 42(29):2089–2102, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2021:CLS

[CJHW21] Jianfu Chen, Menglei Jia, Peijun Hu, and Haifeng Wang. CATKINAS: a large-scale catalytic microkinetic analysis software for mechanism auto-analysis and catalyst screening. *Journal of Computational Chemistry*, 42(5):379–391, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chan:2022:ADC

[CK22] Bun Chan and Amir Karton. Assessment of DLPNO-CCSD(T)-F12 and its use for the formulation of the low-cost and reliable L-W1X composite method. *Journal of Computational Chemistry*, 43(21):1394–1402, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2023:ESP

[CKH23] Siqin Cao, Michael L. Kalin, and Xuhui Huang. `EPISOL`: a software package with expanded functions to perform 3D-RISM calculations for the solvation of chemical and biological molecules. *Journal of Computational Chemistry*, 44(17):1536–1549, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2023:DSC

[CL23] Hsing-Yin Chen and Yu-Fen Lin. DFT study on the catalytic decomposition of hydrogen peroxide by iron complexes of nitrilotriacetate. *Journal of Computational Chemistry*, 44(26): 2058–2072, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cai:2020:SFF

[CLS+20] Yufeng Cai, Xiongjun Li, Zhe Sun, Yutong Lu, Huiying Zhao, Jack Hanson, Kuldip Paliwal, Thomas Litfin, Yaoqi Zhou, and Yuedong Yang. SPOT-Fold: Fragment-free protein structure prediction guided by predicted backbone structure and contact map. *Journal of Computational Chemistry*, 41(8):745–750, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cardenas:2023:MTS

[CLTMd+23] Gustavo Cárdenas, Jesús Lucia-Tamudo, Henar Mateo-delaFuente, Vito F. Palmisano, Nuria Anguita-Ortiz, Lorena Ruano, Álvaro Pérez-Barcia, Sergio Díaz-Tendero, Marcos Mandado, and Juan J. Nogueira. MoBioTools: a toolkit to setup quantum mechanics/molecular mechanics calculations. *Journal of Computational Chemistry*, 44(4):516–533, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chaparro:2020:PPB

[CM20a] Gustavo Chaparro and Andrés Mejía. Phasepy: a Python based framework for fluid phase equilibria and interfacial properties computation. *Journal of Computational Chemistry*, 41 (29):2504–2526, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choudhuri:2020:SBB

[CM20b] Kesaban Sankar Roy Choudhuri and Seema Mishra. Structural basis of BMP-2 and BMP-7 interactions with antagonists Gremlin-1 and Noggin in Glioblastoma tumors. *Journal of Computational Chemistry*, 41(30):2544–2561, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Choudhary:2022:DFT

[CMD+22] Vineet Kumar Choudhary, Kanika Mandhan, Dibyajit Dash, Sachin Bhardwaj, Meena Kumari, and Neeraj Sharma. Density functional theory studies on molecular geometry, spectroscopy, HOMO-LUMO and reactivity descriptors of titanium(IV) and oxidozirconium(IV) complexes of phenylacetohydroxamic acid. *Journal of Computational Chemistry*, 43 (31):2060–2071, December 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Calcagno:2024:MSE

[CMG+24] Francesco Calcagno, Boris Maryasin, Marco Garavelli, Davide Avagliano, and Ivan Rivalta. Modeling solvent effects and convergence of ^{31}P-NMR shielding calculations with COBRAMM. *Journal of Computational Chemistry*, 45(18):1562–1575, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chagas:2024:MDA

[CMO+24] Julio C. V. Chagas, Bruno D. Milanez, Vytor P. Oliveira, Max Pinheiro Jr, Luiz F. A. Ferrão, Adelia J. A. Aquino, Hans Lischka, and Francisco B. C. Machado. A multi-descriptor analysis of substituent effects on the structure and aromaticity of benzene derivatives: π-conjugation versus charge effects. *Journal of Computational Chemistry*, 45(12):863–877, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chilkuri:2021:CMP

[CN21] Vijay Gopal Chilkuri and Frank Neese. Comparison of many-particle representations for selected-CI I: a tree based approach. *Journal of Computational Chemistry*, 42(14):982–1005, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cehic:2023:RHA

[ĆNF23] Mirsada Ćehić and Ivana Niksić-Franjić. Reactions of a hydrogen atom with haloacetates in aqueous solutions: Computational evidence for proton-coupled electron transfer and competing mechanisms. *Journal of Computational Chemistry*, 44 (28):2212–2222, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Conti:2022:PAM

[COK22] Simone Conti, Victor Ovchinnikov, and Martin Karplus. `ppdx`: Automated modeling of protein-protein interaction descriptors for use with machine learning. *Journal of Computational Chemistry*, 43(25):1747–1757, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chevreau:2023:PIP

[CP23] Hilaire Chevreau and Julien Pilmé. Promising insights in parallel grid-based algorithms for quantum chemical topology. *Journal of Computational Chemistry*, 44(16):1505–1516, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casanova-Paez:2021:GDH

[CPG21] Marcos Casanova-Páez and Lars Goerigk. Global double hybrids do not work for charge transfer: a comment on "Double hybrids and time-dependent density functional theory: an implementation and benchmark on charge transfer excited states". *Journal of Computational Chemistry*, 42(8):528–533, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [OMC+20].

Cocic:2022:IWS

[ĆPP+22] Dusan Ćo'cić, Biljana Petrović, Ralph Puchta, Marta Chrzanowska, Anna Katafias, and Rudi van Eldik. Investigation of water substitution at Ru^{II} complexes by conceptual density function theory approach. *Journal of Computational Chemistry*, 43(17):1161–1175, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2020:SCC

[CQSG20] Xin Chen, Zexing Qu, Bingbing Suo, and Jiali Gao. A self-consistent Coulomb bath model using density fitting. *Journal of Computational Chemistry*, 41(18):1698–1708, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Csizi:2024:APN

[CR24] Katja-Sophia Csizi and Markus Reiher. Automated preparation of nanoscopic structures: Graph-based sequence analysis, mismatch detection, and pH-consistent protonation with uncertainty estimates. *Journal of Computational Chemistry*, 45 (11):761–776, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cuesta:2021:CSR

[CRT+21] Sebastián Adolfo Cuesta, Luis Rincón, F. Javier Torres, Vladimir Rodríguez, and José Ramón Mora. A computational study of the reaction mechanism involved in the fast cleavage of an unconstrained amide bond assisted by an amine intramolecular nucleophilic attack. *Journal of Computational Chemistry*, 42(12):818–826, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chamkin:2020:DDC

[CS20] Aleksandr A. Chamkin and Elena S. Serkova. DFT, DLPNO-CCSD(T), and NEVPT2 benchmark study of the reaction between ferrocenium and trimethylphosphine. *Journal of Computational Chemistry*, 41(28):2388–2397, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cerezo:2023:FVR

[CS23] Javier Cerezo and Fabrizio Santoro. `FCclasses3`: Vibrationally-resolved spectra simulated at the edge of the harmonic approximation. *Journal of Computational Chemistry*, 44(4):626–643, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chirico:2021:PQC

[CSG+21] Nicola Chirico, Alessandro Sangion, Paola Gramatica, Linda Bertato, Ilaria Casartelli, and Ester Papa. `QSARINS-Chem` standalone version: a new platform-independent software to profile chemicals for physico-chemical properties, fate, and toxicity. *Journal of Computational Chemistry*, 42(20):1452–1460, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Casals-Sainz:2020:EII

[CSGVF+20] José Luis Casals-Sainz, José Manuel Guevara-Vela, Evelio Francisco, Tomás Rocha-Rinza, and Ángel Martín Pendás. Efficient implementation of the interacting quantum atoms energy partition of the second-order Møller-Plesset energy. *Jour-*

nal of Computational Chemistry, 41(13):1234–1241, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chinnasamy:2020:IBM

[CSP20] Kalaiarasi Chinnasamy, Manjula Saravanan, and Kumaradhas Poomani. Investigation of binding mechanism and downregulation of elacestrant for wild and L536S mutant estrogen receptor-α through molecular dynamics simulation and binding free energy analysis. *Journal of Computational Chemistry*, 41(2):97–109, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cordina:2023:TMP

[CST23] Robert J. Cordina, Beccy Smith, and Tell Tuttle. Triacylglyceride melting point determination using coarse-grained molecular dynamics. *Journal of Computational Chemistry*, 44(21): 1795–1801, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2020:TLC

[CSWW20] Jiu-Li Chen, Tao Sun, Yi-Bo Wang, and Weizhou Wang. Toward a less costly but accurate calculation of the CCSD(T)/CBS noncovalent interaction energy. *Journal of Computational Chemistry*, 41(13):1252–1260, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Contreras-Torres:2020:DCD

[CTBB20] Flavio F. Contreras-Torres, Elena V. Basiuk, and Vladimir A. Basiuk. A dispersion-corrected density functional theory study of the noncovalent interactions between nucleobases and carbon nanotube models containing stone-wales defects. *Journal of Computational Chemistry*, 41(8):780–789, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Corzo:2022:UPO

[CTPJH22] Hector H. Corzo, Ali Abou Taka, Aurora Pribram-Jones, and Hrant P. Hratchian. Using projection operators with maximum overlap methods to simplify challenging self-consistent field optimization. *Journal of Computational Chemistry*, 43 (6):382–390, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Carvalho:2022:CAR

[CV22] Jhonatas R. Carvalho and Luciano N. Vidal. Calculation of absolute Raman scattering cross-sections using vibrational self-consistent field/vibrational configuration interaction wave functions. *Journal of Computational Chemistry*, 43(22):1484–1494, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Castor-Villegas:2020:SHB

[CVGVN+20] Víctor Manuel Castor-Villegas, José Manuel Guevara-Vela, Wilmer E. Vallejo Narváez, Ángel Martín Pendás, Tomás Rocha-Rinza, and Alberto Fernández-Alarcón. On the strength of hydrogen bonding within water clusters on the coordination limit. *Journal of Computational Chemistry*, 41 (26):2266–2277, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Cao:2020:DFS

[CWZD20] Xiaoyan Cao, Liangliang Wu, Jun Zhang, and Michael Dolg. Density functional studies of coenzyme NADPH and its oxidized form $NADP^+$: Structures, UV-Vis spectra, and the oxidation mechanism of NADPH. *Journal of Computational Chemistry*, 41(4):305–316, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chao:2021:CI

[CX21a] Zhen Chao and Dexuan Xie. Cover image. *Journal of Computational Chemistry*, 42(27):i, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chao:2021:IPN

[CX21b] Zhen Chao and Dexuan Xie. An improved Poisson–Nernst–Planck ion channel model and numerical studies on effects of boundary conditions, membrane charges, and bulk concentrations. *Journal of Computational Chemistry*, 42(27):1929–1943, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Chen:2023:DUM

[CX23] Bozhu Chen and Xin Xu. Discriminating and understanding molecular crystal polymorphism. *Journal of Computational*

Chemistry, 44(9):969–979, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dubrovin:2022:CPE

[DA22] Vasilii Dubrovin and Stanislav M. Avdoshenko. Conformational preferences of endohedral metallofullerenes on Ag, Au, and MgO surfaces: Theoretical studies. *Journal of Computational Chemistry*, 43(24):1614–1620, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeSimone:2021:PPH

[DART21] Bruna Clara De Simone, Marta Erminia Alberto, Nino Russo, and Marirosa Toscano. Photophysical properties of heavy atom containing tetrasulfonyl phthalocyanines as possible photosensitizers in photodynamic therapy. *Journal of Computational Chemistry*, 42(25):1803–1808, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deAraujo:2023:HCN

[dARW+23] Luis Octavio de Araujo, Celso R. C. Rêgo, W. Wenzel, Danilo N. Silveira, Maurício J. Piotrowski, Fernando P. Sabino, Yohanes Pramudya, and Diego Guedes-Sobrinho. How cation nature controls the bandgap and bulk Rashba splitting of halide perovskites. *Journal of Computational Chemistry*, 44(14):1395–1403, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Santos:2021:CBH

[dASRHB21] Lucas de Azevedo Santos, Prof. Dr. Teodorico C. Ramalho, Dr. Trevor A. Hamlin, and Prof. Dr. F. Matthias Bickelhaupt. Chalcogen bonds: Hierarchical ab initio benchmark and density functional theory performance study. *Journal of Computational Chemistry*, 42(10):688–698, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dey:2023:APP

[DB23] Priya Dey and Parbati Biswas. Aggregation propensities of proteins with varying degrees of disorder. *Journal of Computational Chemistry*, 44(8):874–886, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deBeer:2020:CBM

[dBCdL20] Shane de Beer, Ignacy Cukrowski, and Jurgens H. de Lange. Characterization of bonding modes in metal complexes through electron density cross-sections. *Journal of Computational Chemistry*, 41(32):2695–2706, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Domnin:2020:FPC

[DBE20] Anton V. Domnin, Andrei V. Bandura, and Robert A. Evarestov. First-principles calculations of phonons and thermodynamic properties of Zr(Hf)S_2-based nanotubes. *Journal of Computational Chemistry*, 41(8):759–768, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Das:2022:CCH

[DC22a] Prasenjit Das and Pratim Kumar Chattaraj. $CSiGaAl_2^{-/0}$ and $CGeGaAl_2^{-/0}$ having planar tetracoordinate carbon atoms in their global minimum energy structures. *Journal of Computational Chemistry*, 43(13):894–905, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dekany:2022:BIP

[DC22b] Attila Á. Dékány and Gábor Czakó. Benchmark ab initio proton affinity and gas-phase basicity of α-alanine based on coupled-cluster theory and statistical mechanics. *Journal of Computational Chemistry*, 43(1):19–28, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Monteiro-de-Castro:2023:HAS

[dCB23] Gabriel Monteiro de Castro and Itamar Borges, Jr. A Hammett's analysis of the substituent effect in functionalized diketopyrrolopyrrole (DPP) systems: Optoelectronic properties and intramolecular charge transfer effects. *Journal of Computational Chemistry*, 44(29):2256–2273, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

delCastillo:2021:IGA

[dCRM21] Roxana M. del Castillo, Estrella Ramos, and Ana Martínez. Interaction of graphene with antipsychotic drugs: Is there any charge transfer process? *Journal of Computational Chemistry*, 42(1):60–65, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

deCarvalho:2020:VTS

[dCVARN20] Edson F. V. de Carvalho, Guilherme D. Vicentini, Tiago Vinicius Alves, and Orlando Roberto-Neto. Variational transition state theory rate constants and H/D kinetic isotope effects for CH_3 + CH_3OCOH reactions. *Journal of Computational Chemistry*, 41(3):231–239, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Das:2023:BSE

[DDSM23] Sujit Das, Kavita Devi, Sonam Suthar, and Kartik Chandra Mondal. Bonding and stability of elusive silaboryne ($Si \equiv B$) and germaboryne ($Ge \equiv B$) with donor base ligands. *Journal of Computational Chemistry*, 44(19):1673–1689, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dare:2022:CRQ

[DF22] Joyce K. Daré and Matheus P. Freitas. Is conformation relevant for QSAR purposes? 2D chemical representation in a 3D-QSAR perspective. *Journal of Computational Chemistry*, 43(13):917–922, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Devi:2022:ENA

[DGM22] Kavita Devi, Sai Manoj N. V. T. Gorantla, and Kartik Chandra Mondal. EDA-NOCV analysis of carbene-borylene bonded dinitrogen complexes for deeper bonding insight: a fair comparison with a metal-dinitrogen system. *Journal of Computational Chemistry*, 43(11):757–777, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Das:2024:AML

[DGS24] Manajit Das, Ankit Ghosh, and Raghavan B. Sunoj. Advances in machine learning with chemical language models in molecular property and reaction outcome predictions. *Journal of Computational Chemistry*, 45(14):1160–1176, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Douglas-Gallardo:2020:ESB

[DGSB+20] Oscar A. Douglas-Gallardo, Ian Shepherd, Simon J. Bennie, Kara E. Ranaghan, Adrian J. Mulholland, and Esteban Vöhringer-Martinez. Electronic structure benchmark calculations of CO_2 fixing elementary chemical steps in RuBisCO using the projector-based embedding approach. *Journal of Computational Chemistry*, 41(24):2151–2157, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Donyapour:2021:CPU

[DHD21] Nazanin Donyapour, Matthew Hirn, and Alex Dickson. `ClassicalGSG`: Prediction of $\log P$ using classical molecular force fields and geometric scattering for graphs. *Journal of Computational Chemistry*, 42(14):1006–1017, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dong:2021:DHP

[DHN+21] Hieu C. Dong, Thi H. Ho, Thu M. Nguyen, Yoshiyuki Kawazoe, and Hung M. Le. Dissociation of hydrogen peroxide in water and methanol through a biased molecular dynamics investigation. *Journal of Computational Chemistry*, 42(19):1344–1353, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dobrovolskiy:2023:TDS

[DK23] Ivan N. Dobrovolskiy and Victor V. Kostjukov. TD-DFT study of BIPS spiropyran: Effects of functionals and high-polarity solvent on C_{spiro}–O bond dissociation and recovery. *Journal of Computational Chemistry*, 44(24):1928–1940, September 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DiGrande:2023:ATA

[DKB23] S. Di Grande, M. Kállay, and V. Barone. Accurate thermochemistry at affordable cost by means of an improved version of the JunChS-F12 model chemistry. *Journal of Computational Chemistry*, 44(27):2149–2157, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dong:2023:EZL

[DLH+23] Shizhi Dong, Yanshuai Li, Hongyu Hu, Ruichuan Li, Bing Yan, Xing Zhang, Zeliang Wang, Jinyu Zhang, and Lin Guo. Effect of ZrS_2 load single/dual-atom catalysts on the hydrogen evolution reaction: a first-principles study. *Journal of Computational Chemistry*, 44(1):15–26, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borba:2024:ABS

[dMBdAVdS24] João Ricardo Bueno de Morais Borba, Leonardo Pereira de Araújo, Marcia Paranho Veloso, and Nelson José Freitas da Silveira. Applying the bioisosterism strategy to obtain lead compounds against SARS-CoV-2 cysteine proteases: an insilico approach. *Journal of Computational Chemistry*, 45(1): 35–46, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DeFever:2021:MCC

[DMD+21] Ryan S. DeFever, Ray A. Matsumoto, Alexander W. Dowling, Peter T. Cummings, and Edward J. Maginn. MoSDeF Cassandra: a complete Python interface for the Cassandra Monte Carlo software. *Journal of Computational Chemistry*, 42(18): 1321–1331, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simone:2022:OPA

[DMTR22] Bruna Clara De Simone, Gloria Mazzone, Marirosa Toscano, and Nino Russo. On the origin of photodynamic activity of hypericin and its iodine-containing derivatives. *Journal of Computational Chemistry*, 43(30):2037–2042, November 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Diem:2020:EDC

[DO20] Matthias Diem and Chris Oostenbrink. The effect of different cutoff schemes in molecular simulations of proteins. *Journal of Computational Chemistry*, 41(32):2740–2749, December 15,

2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dorofeeva:2020:APN

[Dor20] Olga V. Dorofeeva. Accurate prediction of norbornadiene cycle enthalpies by DLPNO-CCSD(T_1)/CBS method. *Journal of Computational Chemistry*, 41(27):2352–2364, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Duzenli:2022:IGE

[DOT22] Derya Düzenli, Isik Onal, and Ilker Tezsevin. Investigation of glucose electrooxidation mechanism over *N*-modified metal-doped graphene electrode by density functional theory approach. *Journal of Computational Chemistry*, 43(26):1793–1801, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Devillers:2020:CDP

[DPSG20] Marion Devillers, Jean-Philip Piquemal, Laurent Salmon, and Nohad Gresh. Calibration of the dianionic phosphate group: Validation on the recognition site of the homodimeric enzyme phosphoglucose isomerase. *Journal of Computational Chemistry*, 41(8):839–854, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dong:2022:PXB

[DPY+22] Jing Dong, Lichao Peng, Xiaohui Yang, Zelin Zhang, and Puyu Zhang. `XGBoost`-based intelligence yield prediction and reaction factors analysis of amination reaction. *Journal of Computational Chemistry*, 43(4):289–302, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

DAnania:2024:PPS

[DRBT24] Olga D'Anania, Eugenio Romano, Vincenzo Barone, and Giovanni Talarico. Predicting the propene stereoselectivity on transition metal catalysts: a daunting task for density functional theory. *Journal of Computational Chemistry*, 45(17): 1483–1492, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Santos:2021:CI

[dRHB21] Lucas de Azevedo Santos, Teodorico C. Ramalho, Trevor A. Hamlin, and F. Matthias Bickelhaupt. Cover image. *Journal of Computational Chemistry*, 42(10):C1, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dubey:2023:IFM

[DSB23] Gurudutt Dubey, Tejender Singh, and Prasad V. Bharatam. The importance of four-membered NHCs in stabilizing breslow intermediates on benzoin condensation pathway. *Journal of Computational Chemistry*, 44(3):346–354, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

daSilva:2020:TTA

[dSBFdAJ20] Amauri Duarte da Silva, Gabriela Bitencourt-Ferreira, and Walter Filgueira de Azevedo Jr. Taba: a tool to analyze the binding affinity. *Journal of Computational Chemistry*, 41(1): 69–73, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Das:2020:EMI

[DSC20] Prasenjit Das, Ranajit Saha, and Pratim K. Chattaraj. Encapsulation of Mg_2 inside a C_{60} cage forms an electride. *Journal of Computational Chemistry*, 41(17):1645–1653, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dias-da-Silva:2021:EBT

[dSCCN21] Gabriela Dias da Silva, Rodrigo L. O. R. Cunha, and Mauricio D. Coutinho-Neto. Equilibrium between tri- and tetracoordinate chalcogenuranes is critical for cysteine protease inhibition. *Journal of Computational Chemistry*, 42(17):1225–1235, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dutta:2021:RDP

[DSK21] Moumita Dutta, Hemant Kumar Srivastava, and Akshai Kumar. Rational design of pincer-nickel complexes for catalytic cyanomethylation of benzaldehyde: a systematic DFT study. *Journal of Computational Chemistry*, 42(24):1728–

1735, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dabbish:2024:ICM

[DSS+24] Eslam Dabbish, Stefano Scoditti, Mohammed N. I. Shehata, Ida Ritacco, Mahmoud A. A. Ibrahim, Tamer Shoeib, and Emilia Sicilia. Insights on cyclophosphamide metabolism and anticancer mechanism of action: a computational study. *Journal of Computational Chemistry*, 45(10):663–670, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silva:2024:EQE

[dSSCC24] Lucas de S. Silva, Guilherme Colherinhas, and Wesley B. Cardoso. Evaluating quantum entanglement generation in two-dimensional graphene systems through lithium ion interactions: a DFT-based study. *Journal of Computational Chemistry*, 45(13):1002–1007, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Silva:2024:PFI

[dSSRVdM24] Albert J. F. W. H. de S. Silva, Gessenildo P. Rodrigues, Elizete Ventura, and Silmar A. do Monte. Photodissociation and formation of an ion-pair in CH_2 FCl (HCFC-31). *Journal of Computational Chemistry*, 45(8):476–486, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Doi:2021:SLO

[DTA21] Hideo Doi, Kazuaki Z. Takahashi, and Takeshi Aoyagi. Searching for local order parameters to classify water structures at triple points. *Journal of Computational Chemistry*, 42(24):1720–1727, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ding:2020:EEP

[DWSX20] Chen Ding, Jingwei Weng, Tonghao Shen, and Xin Xu. The enhanced extended phenomenological kinetics method to deal with timescale disparity problem among different reaction pathways. *Journal of Computational Chemistry*, 41(24):2115–2123, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dang:2022:NES

[DWZ22] Duy-Khoi Dang, Leighton W. Wilson, and Paul M. Zimmerman. The numerical evaluation of Slater integrals on graphics processing units. *Journal of Computational Chemistry*, 43(25): 1680–1689, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Druchok:2021:TEG

[DYGM21] Maksym Druchok, Dzvenymyra Yarish, Oleksandr Gurbych, and Mykola Maksymenko. Toward efficient generation, correction, and properties control of unique drug-like structures. *Journal of Computational Chemistry*, 42(11):746–760, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Deng:2023:AAR

[DZ23] Qianqian Deng and Jun Zhu. Adaptive σ aromaticity in the rhenacyclopropene rings. *Journal of Computational Chemistry*, 44(29):2294–2301, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Damte:2020:BCD

[DZL+20] Jemal Yimer Damte, Zhan-Jun Zhu, Pin-Jun Lin, Chen-Hao Yeh, and Jyh-Chiang Jiang. B, N-co-doped graphene-supported Ir and Pt clusters for methane activation and C–C coupling: a density functional theory study. *Journal of Computational Chemistry*, 41(3):194–202, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eisele:2020:MMK

[EG20] Sebastian Eisele and Steffen Grieshammer. MOCASSIN: Metropolis and kinetic Monte Carlo for solid electrolytes. *Journal of Computational Chemistry*, 41(31):2663–2677, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Efaz:2021:RFI

[EIT+21] Faiyaz Md. Efaz, Shafiqul Islam, Shafi Ahmad Talukder, Shaila Akter, Md. Zakaria Tashrif, Md. Ackas Ali, Md. Abu Sufian, Md. Rimon Parves, Md. Jahirul Islam, and Mohammad A. Halim. Repurposing fusion inhibitor peptide against

SARS-CoV-2. *Journal of Computational Chemistry*, 42(32): 2283–2293, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ehlert:2020:PPP

[EK20a] Christopher Ehlert and Tillmann Klamroth. PSIXAS: a Psi4 plugin for efficient simulations of X-ray absorption spectra based on the transition-potential and Δ-Kohn–Sham method. *Journal of Computational Chemistry*, 41(19):1781–1789, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2020:OPI

[EK20b] Robert A. Evarestov and Alexei Kuzmin. Origin of pressure-induced insulator-to-metal transition in the van der Waals compound $FePS_3$ from first-principles calculations. *Journal of Computational Chemistry*, 41(14):1337–1344, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2020:TAC

[EK20c] Robert A. Evarestov and Alexei Kuzmin. Topological analysis of chemical bonding in the layered $FePSe_3$ upon pressure-induced phase transitions. *Journal of Computational Chemistry*, 41(31):2610–2623, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Edholm:2024:PEA

[ENR+24] Freya Edholm, Aditya Nandy, Clorice R. Reinhardt, David W. Kastner, and Heather J. Kulik. Protein3D: Enabling analysis and extraction of metal-containing sites from the Protein Data Bank with molSimplify. *Journal of Computational Chemistry*, 45(6):352–361, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Evarestov:2021:AIA

[EPT21] Robert A. Evarestov, Andrej I. Panin, and Yuri S. Tverjanovich. Argentophillic interactions in argentum chalcogenides: First principles calculations and topological analysis of electron density. *Journal of Computational Chemistry*, 42(4):242–247, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Egorov:2024:AIP

[ERVN24] Oleg Egorov, Michaël Rey, Dominika Viglaska, and Andrei V. Nikitin. Accurate ab initio potential energy surface, rovibrational energy levels and resonance interactions of triplet ($^3B_1$) methylene. *Journal of Computational Chemistry*, 45(2):83–100, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ebisawa:2021:CI

[ETT21a] Shuichi Ebisawa, Takuro Tsutsumi, and Tetsuya Taketsugu. Cover image. *Journal of Computational Chemistry*, 42(1):i, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ebisawa:2021:GAA

[ETT21b] Shuichi Ebisawa, Takuro Tsutsumi, and Tetsuya Taketsugu. Geometric analysis of anharmonic downward distortion following paths. *Journal of Computational Chemistry*, 42(1):27–39, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Eidi:2021:HOH

[EVKL21] Mohammadreza Eidi, Mohsen Vafaee, Hamed Koochaki Kelardeh, and Alexandra Landsman. High-order harmonic generation by static coherent states method in single-electron atomic and molecular systems. *Journal of Computational Chemistry*, 42(18):1312–1320, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Freindorf:2024:IHB

[FAK24] Marek Freindorf, Juliana J. Antonio, and Elfi Kraka. Iron-histidine bonding in bishistidyl hemoproteins — a local vibrational mode study. *Journal of Computational Chemistry*, 45 (9):574–588, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fouda:2020:IPQ

[FB20] Adam A. E. Fouda and Nicholas A. Besley. Improving the predictive quality of time-dependent density functional theory calculations of the X-ray emission spectroscopy of organic molecules. *Journal of Computational Chemistry*, 41(11):1081–

1090, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feldt:2021:ALC

[FB21] Milica Feldt and Alex Brown. Assessment of local coupled cluster methods for excited states of BODIPY/Aza-BODIPY families. *Journal of Computational Chemistry*, 42(3):144–155, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Felix:2023:MAC

[FBM+23] João P. C. S. Felix, Krys E. A. Batista, Wesley O. Morais, Glaucio R. Nagurniak, Renato P. Orenha, Celso R. C. Rêgo, Diego Guedes-Sobrinho, Renato L. T. Parreira, Mateus M. Ferrer, and Maurício J. Piotrowski. Molecular adsorption on coinage metal subnanoclusters: a DFT+D3 investigation. *Journal of Computational Chemistry*, 44(10):1040–1051, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fukal:2022:AMM

[FBP+22] Jirí Fukal, Milos Budesínský, Ondrej Páv, Petr Jurecka, Marie Zgarbová, Jakub Sebera, and Vladimír Sychrovský. The Ad-MD method to calculate NMR shift including effects due to conformational dynamics: The ^{31}P NMR shift in DNA. *Journal of Computational Chemistry*, 43(2):132–143, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fatkova:2023:VEE

[FCB23] Katerina Fatková, Radim Cajzl, and Jaroslav V. Burda. The vertical excitation energies and a lifetime of the two lowest singlet excited states of the conjugated polyenes from C2 to C22: Ab initio, DFT, and semiclassical MNDO-MD simulations. *Journal of Computational Chemistry*, 44(6):777–787, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fregoni:2020:PSC

[FCPG20] Jacopo Fregoni, Stefano Corni, Maurizio Persico, and Giovanni Granucci. Photochemistry in the strong coupling regime: a trajectory surface hopping scheme. *Journal of Computational Chemistry*, 41(23):2033–2044, September 5, 2020.

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

Fan:2023:SSP

[FDD+23] Dan Fan, Juan Du, Jingshuang Dang, Changwei Wang, and Yirong Mo. The strength and selectivity of perfluorinated nano-hoops and buckybowls for anion binding and the nature of anion-π interactions. *Journal of Computational Chemistry*, 44(3):138–148, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Freindorf:2022:CBH

[FDK22] Marek Freindorf, Alexis Antoinette Ann Delgado, and Elfi Kraka. CO bonding in hexa- and pentacoordinate carboxyneuroglobin: a quantum mechanics/molecular mechanics and local vibrational mode study. *Journal of Computational Chemistry*, 43(25):1725–1746, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fedorov:2022:PEF

[Fed22] Dmitri G. Fedorov. Polarization energies in the fragment molecular orbital method. *Journal of Computational Chemistry*, 43(16):1094–1103, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fedorov:2024:UCA

[Fed24] Dmitri G. Fedorov. Use of caps in the auxiliary basis set formulation of the fragment molecular orbital method. *Journal of Computational Chemistry*, 45(18):1540–1551, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujimori:2021:EBA

[FKT21] Toshikazu Fujimori, Masato Kobayashi, and Tetsuya Taketsugu. Energy-based automatic determination of buffer region in the divide-and-conquer second-order Møller–Plesset perturbation theory. *Journal of Computational Chemistry*, 42(9): 620–629, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Freites:2023:ISD

[FLT23] J. Alfredo Freites, Mohab N. Louis, and Douglas J. Tobias. Insights into the solubility of γ D-crystallin from multiscale atomistic simulations. *Journal of Computational Chemistry*, 44(19):1658–1666, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Frazee:2021:IIP

[FM21] Nicolas Frazee and Blake Mertz. Intramolecular interactions play key role in stabilization of pHLIP at acidic conditions. *Journal of Computational Chemistry*, 42(25):1809–1816, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fiorin:2020:DDF

[FMFG20] Giacomo Fiorin, Fabrizio Marinelli, and José D. Faraldo-Gómez. Direct derivation of free energies of membrane deformation and other solvent density variations from enhanced sampling molecular dynamics. *Journal of Computational Chemistry*, 41(5):449–459, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Filatov:2024:UEA

[FMK24] Michael Filatov, Vladimir Mironov, and Elfi Kraka. Unraveling the effect of aromaticity for the dynamics of excited states of single benzene fluorophores. *Journal of Computational Chemistry*, 45(13):1033–1045, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fernandez:2022:BSI

[FNPD22] Israel Fernández, Anurag Noonikara-Poyil, and H. V. Rasika Dias. Bonding situation in isolable silver(I) carbonyl complexes of the Scorpionates. *Journal of Computational Chemistry*, 43(11):796–803, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fujimoto:2021:MRO

[FNY21] Kazushi Fujimoto, Tetsuro Nagai, and Tsuyoshi Yamaguchi. Momentum removal to obtain the position-dependent diffusion constant in constrained molecular dynamics simulation. *Journal of Computational Chemistry*, 42(30):2136–2144, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Faizan:2022:BBI

[FP22] Mohmmad Faizan and Ravinder Pawar. Boron based intramolecular heterocyclic frustrated Lewis pairs as organocatalysts for CO_2 adsorption and activation. *Journal of Computational Chemistry*, 43(22):1474–1483, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Faizan:2023:ABA

[FP23] Mohmmad Faizan and Ravinder Pawar. Alanine boronic acid functionalized UiO-66 MOF as a nanoreactor for the conversion of CO_2 into formic acid. *Journal of Computational Chemistry*, 44(18):1624–1633, July 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Feltes:2023:NSV

[FPMD23] Bruno César Feltes, Éderson Sales Moreira Pinto, Arthur Tonietto Mangini, and Márcio Dorn. `NIAS-Server 2.0`: a versatile complementary tool for structural biology studies. *Journal of Computational Chemistry*, 44(18):1610–1623, July 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Flachsenberg:2021:LOS

[FR21] Florian Flachsenberg and Matthias Rarey. `LSLOpt`: An open-source implementation of the step-length controlled LSL-BFGS algorithm. *Journal of Computational Chemistry*, 42 (15):1095–1100, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Forster:2020:DHD

[FV20] Arno Förster and Lucas Visscher. Double hybrid DFT calculations with Slater type orbitals. *Journal of Computational Chemistry*, 41(18):1660–1684, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Friis:2020:MEI

[FVSS20] Ida Friis, Alexey Verkhovtsev, Ilia A. Solov'yov, and Andrey V. Solov'yov. Modeling the effect of ion-induced shock waves and DNA breakage with the reactive CHARMM force field. *Journal of Computational Chemistry*, 41(28):2429–2439, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Fukuhara:2023:IPR

[FYIO23] Daiki Fukuhara, Masataka Yamauchi, Satoru G. Itoh, and Hisashi Okumura. Ingenuity in performing replica permutation: How to order the state labels for improving sampling efficiency. *Journal of Computational Chemistry*, 44(4):534–545, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gutsev:2020:IBD

[GAG20] Lavrenty G. Gutsev, Sergey M. Aldoshin, and Gennady L. Gutsev. Influence of back donation effects on the structure of ZnO nanoclusters. *Journal of Computational Chemistry*, 41(30):2583–2590, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gao:2020:GRR

[Gao20] Bin Gao. General recurrence-relation generation scheme for molecular integral evaluation. *Journal of Computational Chemistry*, 41(32):2722–2739, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Geindre:2021:NLR

[GAP21] Hugo Geindre, Abdul-Rahman Allouche, and Daniel Peláez. Non long-range corrected density functionals incorrectly describe the intensity of the C–H stretching band in polycyclic aromatic hydrocarbons. *Journal of Computational Chemistry*, 42(14):1018–1027, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garnier:2020:FEC

[GBM20] Ludovic Garnier, Christine Bonal, and Patrice Malfreyt. Free-energy calculations of the host-guest association in grafted supramolecular assemblies. *Journal of Computational Chemistry*, 41(25):2189–2196, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gong:2020:AGB

[GCL+20] Xiping Gong, Mara Chiricotto, Xiaorong Liu, Erik Nordquist, Michael Feig, Charles L. Brooks III, and Jianhan Chen. Accelerating the generalized Born with molecular volume and solvent accessible surface area implicit solvent model using graphics processing units. *Journal of Computational Chemistry*, 41 (8):830–838, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gallegos:2022:RSP

[GCP22] Miguel Gallegos, Aurora Costales, and Ángel Martín Pendás. A real space picture of the role of steric effects in S_N2 reactions. *Journal of Computational Chemistry*, 43(11):785–795, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Geerlings:2023:EFC

[GD23] Paul Geerlings and Frank De Proft. External fields in conceptual density functional theory. *Journal of Computational Chemistry*, 44(3):442–455, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gomez:2021:LAF

[GFRNC21] Tatiana Gómez, Patricio Fuentealba, Andrés Robles-Navarro, and Carlos Cárdenas. Links among the Fukui potential, the alchemical hardness and the local hardness of an atom in a molecule. *Journal of Computational Chemistry*, 42(23):1681–1688, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gkogka:2022:FMD

[GG22] Ioanna Gkogka and Nicholas M. Glykos. Folding molecular dynamics simulation of T-peptide, a HIV viral entry inhibitor: Structure, dynamics, and comparison with the experimental data. *Journal of Computational Chemistry*, 43(14):942–952, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghalami:2020:AST

[GGK20] Zahra Ghalami, Vanik Ghoulipour, and Ali Reza Khanchi. Adsorption and sequential thermal release of F_2, Cl_2, and Br_2 molecules by a porous organic cage material (CC3-R): Molecular dynamics and grand-canonical Monte Carlo simulations. *Journal of Computational Chemistry*, 41(9):949–957, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gallmetzer:2022:PRA

[GH22a] Hans Georg Gallmetzer and Thomas S. Hofer. Probing the range of applicability of structure- and energy-adjusted QM/ MM link bonds II: Optimized link bond parameters for density functional tight binding approaches. *Journal of Computational Chemistry*, 43(11):746–756, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gusmao:2022:RAG

[GH22b] Eriosvaldo Florentino Gusmão and Roberto Luiz Andrade Haiduke. Relativistic adapted Gaussian basis sets free of variational prolapse of small and medium size for hydrogen through xenon. *Journal of Computational Chemistry*, 43(28):1901–1910, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gusmao:2023:RAG

[GH23] Eriosvaldo Florentino Gusmão and Roberto Luiz Andrade Haiduke. Relativistic adapted Gaussian basis sets free of variational prolapse of small and medium size for cesium through radon. *Journal of Computational Chemistry*, 44(32):2478–2485, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gieseking:2021:NRM

[Gie21] Rebecca L. M. Gieseking. A new release of MOPAC incorporating the INDO/S semiempirical model with CI excited states. *Journal of Computational Chemistry*, 42(5):365–378, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gui:2021:ELM

[GJL21] Shaojun Gui, Ling Jiang, and Zhi-Feng Liu. Evolution of the linker in microhydrated hydrogen dinitrate anions: From H^+ to $H_5O_2^+$. *Journal of Computational Chemistry*, 42(21):1514–1525, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Jacas:2020:SST

[GJMPB$^+$20] César R. García-Jacas, Yovani Marrero-Ponce, Carlos A. Brizuela, José Suárez-Lezcano, and Felix Martinez-Rios. Smoothed spherical truncation based on fuzzy membership functions: Application to the molecular encoding. *Journal of Computational Chemistry*, 41(3):203–217, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Jacas:2020:DMQ

[GJMPVR+20] César R. García-Jacas, Yovani Marrero-Ponce, Ricardo Vivas-Reyes, José Suárez-Lezcano, Felix Martinez-Rios, Julio E. Terán, and Longendri Aguilera-Mendoza. Distributed and multicore QuBiLS-MIDAS software v2.0: Computing chiral, fuzzy, weighted and truncated geometrical molecular descriptors based on tensor algebra. *Journal of Computational Chemistry*, 41(12):1209–1227, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghysbrecht:2024:TIR

[GK24] Simon Ghysbrecht and Bettina G. Keller. Thermal isomerization rates in retinal analogues using ab-initio molecular dynamics. *Journal of Computational Chemistry*, 45(16):1390–1403, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gorantla:2023:CI

[GKA+23a] Sai Manoj N. V. T. Gorantla, Harsha S. Karnamkkott, Selvakumar Arumugam, Sangita Mondal, and Kartik Chandra Mondal. Cover image. *Journal of Computational Chemistry*, 44(1):i, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gorantla:2023:SBC

[GKA+23b] Sai Manoj N. V. T. Gorantla, Harsha S. Karnamkkott, Selvakumar Arumugam, Sangita Mondal, and Kartik Chandra Mondal. Stability and bonding of carbon(0)-iron-N_2 complexes relevant to nitrogenase co-factor: EDA-NOCV analyses. *Journal of Computational Chemistry*, 44(1):43–60, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Goncalves:2022:SPT

[GKO+22] Yan M. H. Gonçalves, Sadra Kashefolgheta, Marina P. Oliveira, Philippe H. Hünenberger, and Bruno A. C. Horta. Simultaneous parametrization of torsional and third-neighbor interaction terms in force-field development: the LLS-SC algorithm. *Journal of Computational Chemistry*, 43(9):644–653, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gehlhaar:2022:PCS

[GLC+22] Daniel K. Gehlhaar, Brock A. Luty, Philip P. Cheung, Andy H. Litman, Robert M. Owen, and Peter W. Rose. The Pfizer Crystal Structure Database: an essential tool for structure-based design at Pfizer. *Journal of Computational Chemistry*, 43(15):1053–1062, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gorantla:2022:UHR

[GM22] Sai Manoj N. V. T. Gorantla and Kartik Chandra Mondal. Uncovering the hidden reactivity of benzyne/aryne precursors utilized under milder condition: Bonding and stability studies by EDA-NOCV analyses. *Journal of Computational Chemistry*, 43(23):1543–1560, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gerhards:2023:MSR

[GNK+23] Luca Gerhards, Claus Nielsen, Daniel R. Kattnig, P. J. Hore, and Ilia A. Solov'yov. Modeling spin relaxation in complex radical systems using `MolSpin`. *Journal of Computational Chemistry*, 44(19):1704–1714, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gomez:2022:TMC

[GNL+22] Yessica K. Gomez, Andrew M. Natale, James Lincoff, Charles W. Wolgemuth, John M. Rosenberg, and Michael Grabe. Taking the Monte-Carlo gamble: How not to buckle under the pressure! *Journal of Computational Chemistry*, 43 (6):431–434, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Griffiths:2020:AIP

[GOY20] Thomas M. Griffiths, Aaron J. Oakley, and Haibo Yu. Atomistic insights into photoprotein formation: Computational prediction of the properties of coelenterazine and oxygen binding in obelin. *Journal of Computational Chemistry*, 41(6):587–603, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gresh:2021:MCP

[GP21] Nohad Gresh and David Perahia. Multimolecular complexes of the phosphodiester anion with Zn(II) or Mg(II) and water molecules — preliminary validations of a polarizable potential by ab initio quantum chemistry. *Journal of Computational Chemistry*, 42(20):1430–1446, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gentile:2020:SCD

[GPEK+20] Francesco S. Gentile, Alexander Platonenko, Khaled E. El-Kelany, Michel Rérat, Philippe D'Arco, and Roberto Dovesi. Substitutional carbon defects in silicon: a quantum mechanical characterization through the infrared and Raman spectra. *Journal of Computational Chemistry*, 41(17):1638–1644, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gorantla:2021:CI

[GPM21a] Sai Manoj N. V. T. Gorantla, Pattiyil Parameswaran, and Kartik Chandra Mondal. Cover image. *Journal of Computational Chemistry*, 42(16), June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gorantla:2021:SGE

[GPM21b] Sai Manoj N. V. T. Gorantla, Pattiyil Parameswaran, and Kartik Chandra Mondal. Stabilization of group 14 elements E = C, Si, Ge by hetero-bileptic ligands cAAC, MCO_n with push-pull mechanism. *Journal of Computational Chemistry*, 42(16):1159–1177, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Rates:2021:ISD

[GRBN21] Miquel Garcia-Ratés, Ute Becker, and Frank Neese. Implicit solvation in domain based pair natural orbital coupled cluster (DLPNO–CCSD) theory. *Journal of Computational Chemistry*, 42(27):1959–1973, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia-Rates:2020:ESC

[GRN20] Miquel Garcia-Ratés and Frank Neese. Effect of the solute cavity on the solvation energy and its derivatives within the framework of the Gaussian charge scheme. *Journal of Computational Chemistry*, 41(9):922–939, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Geiger:2022:AIS

[GSD+22] Julian Geiger, Volker Settels, Peter Deglmann, Ansgar Schäfer, and Maike Bergeler. Automated input structure generation for single-ended reaction path optimizations. *Journal of Computational Chemistry*, 43(24):1662–1674, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ghiami-Shomami:2023:PCS

[GSH23] Ali Ghiami-Shomami and Christof Hättig. Performance of the COSMO solvation model for photoacidity and basicity in water. *Journal of Computational Chemistry*, 44(24):1941–1955, September 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Guan:2023:DMS

[GSJ+23] Xiao-Ling Guan, Rui Sun, Bo Jin, Caixia Yuan, and Yan-Bo Wu. 3-D molecular stars with covalent axial bonding. *Journal of Computational Chemistry*, 44(15):1410–1417, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grazioli:2024:TPC

[GSSG24] Laura Grazioli, Luca T. Schleicher, Stella Stopkowicz, and Jürgen Gauss. Theoretical prediction of closed-shell paramagnetism for scandium and yttrium hydride. *Journal of Computational Chemistry*, 45(15):1215–1223, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Grillo:2020:SMD

[GUCCR20] Igor Barden Grillo, Gabriel A. Urquiza-Carvalho, Elton José Ferreira Chaves, and Gerd Bruno Rocha. Semiempirical methods do Fukui functions: Unlocking a modeling framework for biosystems. *Journal of Computational Chemistry*, 41(9): 862–873, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gupta:2022:EHD

[GVJ+22] Abhinav Gupta, Shivani Verma, Ramsha Javed, Suraj Sudhakar, Saurabh Srivastava, and Nisanth N. Nair. Exploration of high dimensional free energy landscapes by a combination of temperature-accelerated sliced sampling and parallel biasing. *Journal of Computational Chemistry*, 43(17):1186–1200, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gangopadhyay:2021:ANP

[GWN21] Ananya Gangopadhyay, Simon Winberg, and Kevin J. Naidoo. Anisotropic numerical potentials for coarse-grained modeling from high-speed multidimensional lookup table and interpolation algorithms. *Journal of Computational Chemistry*, 42(10): 666–675, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Gu:2020:EKT

[GX20] Yonghao Gu and Xin Xu. Extended Koopmans' theorem at the second-order perturbation theory. *Journal of Computational Chemistry*, 41(12):1165–1174, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Garcia:2021:POB

[GZFSM21] Victor García, David Zorrilla, Manuel Fernández, and Jesús Sánchez-Márquez. Property-oriented basis sets for computation of atomization energies. *Journal of Computational Chemistry*, 42(30):2154–2162, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hanasaki:2023:FC

[HAC+23a] Kota Hanasaki, Zulfikhar A. Ali, Min Choi, Mauro Del Ben, and Bryan M. Wong. Front cover. *Journal of Computational Chemistry*, 44(9):C1, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hanasaki:2023:IRT

[HAC+23b] Kota Hanasaki, Zulfikhar A. Ali, Min Choi, Mauro Del Ben, and Bryan M. Wong. Implementation of real-time TDDFT for periodic systems in the open-source `PySCF` software package. *Journal of Computational Chemistry*, 44(9):980–987, April 5,

2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayes:2021:SPG

[HB21] Ryan L. Hayes and Charles L. Brooks III. A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. *Journal of Computational Chemistry*, 42 (15):1088–1094, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirakawa:2020:BME

[HBM+20] Teruo Hirakawa, David R. Bowler, Tsuyoshi Miyazaki, Yoshitada Morikawa, and Lionel A. Truflandier. Blue moon ensemble simulation of aquation free energy profiles applied to mono and bifunctional platinum anticancer drugs. *Journal of Computational Chemistry*, 41(22):1973–1984, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoffmann:2020:PEE

[HBT+20] Guillaume Hoffmann, Muhammet Balcilar, Vincent Tognetti, Pierre Héroux, Benoît Gaüzère, Sébastien Adam, and Laurent Joubert. Predicting experimental electrophilicities from quantum and topological descriptors: a machine learning approach. *Journal of Computational Chemistry*, 41(24):2124–2136, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hassan:2021:PSS

[HC21] Mosavverul Hassan and Evangelos A. Coutsias. Protein secondary structure motifs: a kinematic construction. *Journal of Computational Chemistry*, 42(5):271–292, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirao:2020:EEE

[HCS+20] Kimihiko Hirao, Bun Chan, Jong-Won Song, Kamala Bhattarai, and Subrata Tewary. Excitation energies expressed as orbital energies of Kohn–Sham density functional theory with long-range corrected functionals. *Journal of Computational Chemistry*, 41(14):1368–1383, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huang:2022:MSC

[HCY+22] Runfeng Huang, Jiali Cai, Lei Yao, Yuna Bai, Kai Guo, and Lili Zhao. Mechanistic study of cobalt(I)-catalyzed asymmetric coupling of ethylene and enynes to functionalized cyclobutanes. *Journal of Computational Chemistry*, 43(7):440–447, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hoffmann:2021:DES

[HD21] Marvin Hoffmann and Andreas Dreuw. Deciphering excited state properties utilizing algebraic diagrammatic construction schemes of decreasing order. *Journal of Computational Chemistry*, 42(11):793–800, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haase:2020:NDC

[HFPS20] Pi A. B. Haase, Rasmus Faber, Patricio F. Provasi, and Stephan P. A. Sauer. Noniterative doubles corrections to the random phase and higher random phase approximations: Singlet and triplet excitation energies. *Journal of Computational Chemistry*, 41(1):43–55, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hu:2020:RFM

[HGF20] Xiuzhen Hu, Riletu Ge, and Zhenxing Feng. Recognizing five molecular ligand-binding sites with similar chemical structure. *Journal of Computational Chemistry*, 41(2):110–118, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hesselmann:2024:DFI

[HGR+24] Andreas Heßelmann, Emmanuel Giner, Peter Reinhardt, Peter J. Knowles, Hans-Joachim Werner, and Julien Toulouse. A density-fitting implementation of the density-based basis-set correction method. *Journal of Computational Chemistry*, 45(15):1247–1253, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hwang:2020:MMM

[HHL+20] Hyea Hwang, Anthony Hazel, Peng Lian, Jeremy C. Smith, James C. Gumbart, and Jerry M. Parks. A minimal membrane metal transport system: Dynamics and energetics of mer proteins. *Journal of Computational Chemistry*, 41(6):528–537, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haghshenas:2021:DVQ

[HKFT21] Hamed Haghshenas, Bita Kaviani, Monireh Firouzeh, and Hossein Tavakol. Developing a variation of 3D-QSAR/MD method in drug design. *Journal of Computational Chemistry*, 42(13):917–929, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Harding:2020:IMS

[HKSW20] Drew P. Harding, Laura J. Kingsley, Glen Spraggon, and Steven E. Wheeler. Importance of model size in quantum mechanical studies of DNA intercalation. *Journal of Computational Chemistry*, 41(12):1175–1184, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Han:2020:CAS

[HL20] Ruocheng Han and Sandra Luber. Complete active space analysis of a reaction pathway: Investigation of the oxygen-oxygen bond formation. *Journal of Computational Chemistry*, 41(17): 1586–1597, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Huynh:2024:SML

[HLV+24] Hieu Huynh, Khanh Le, Linh Vu, Trang Nguyen, Matthew Holcomb, Stefano Forli, and Hung Phan. Synergy of machine learning and density functional theory calculations for predicting experimental Lewis base affinity and Lewis polybase binding atoms. *Journal of Computational Chemistry*, 45(18): 1552–1561, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Henkel:2021:UEC

[HM21] Pascal Henkel and Doreen Mollenhauer. Uncertainty of exchange-correlation functionals in density functional theory calculations for lithium-based solid electrolytes on the case study of lithium phosphorus oxynitride. *Journal of Computational Chemistry*, 42(18):1283–1295, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haasler:2023:TCT

[HMK23] Matthias Haasler, Toni M. Maier, and Martin Kaupp. Toward a correct treatment of core properties with local hybrid functionals. *Journal of Computational Chemistry*, 44(32):2461–2477, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hirao:2024:VDS

[HNCL24] Kimihiko Hirao, Takahito Nakajima, Bun Chan, and Ho-Jin Lee. The verification of delta SCF and Slater's transition state theory for the calculation of core ionization energy. *Journal of Computational Chemistry*, 45(3):183–192, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hernandez:2020:AIM

[HPG20] Belén Hernández, Fernando Pflüger, and Mahmoud Ghomi. Aspartate: An interesting model for analyzing dipole–ion and ion pair interactions through its oppositely charged amine and acid groups. *Journal of Computational Chemistry*, 41(14):1402–1410, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hutcheson:2021:DGE

[HPM+21] Anders Hutcheson, Alexander Christian Paul, Rolf H. Myhre, Henrik Koch, and Ida-Marie Høyvik. Describing ground and excited state potential energy surfaces for molecular photoswitches using coupled cluster models. *Journal of Computational Chemistry*, 42(20):1419–1429, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hernandez-Rodriguez:2020:MSS

[HREvdK+20] Erix W. Hernández-Rodríguez, Andrés M. Escorcia, Marc W. van der Kamp, Ana L. Montero-Alejo, and Julio Caballero. Multi-scale simulation reveals that an amino acid substitution increases photosensitizing reaction inputs in rhodopsins. *Journal of Computational Chemistry*, 41(26):2278–2295, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hughes:2020:FWM

[HRT+20] Zak E. Hughes, Emmanuel Ren, Joseph C. R. Thacker, Benjamin C. B. Symons, Arnaldo F. Silva, and Paul L. A. Popelier. A FFLUX water model: Flexible, polarizable and with a multipolar description of electrostatics. *Journal of Computational Chemistry*, 41(7):619–628, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hidalgo-Rosa:2020:SME

[HRTSS+20] Yoan Hidalgo-Rosa, Manuel A. Treto-Suárez, Eduardo Schott, Ximena Zarate, and Dayán Páez-Hernández. Sensing mechanism elucidation of a europium(III) metal-organic framework selective to aniline: a theoretical insight by means of multiconfigurational calculations. *Journal of Computational Chemistry*, 41(22):1956–1964, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haritha:2022:HPR

[HS22] Mambatta Haritha and Cherumuttathu H. Suresh. Hydration patterns of rings in drugs and relationship to lipophilicity: a DFT study. *Journal of Computational Chemistry*, 43(7):477–490, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Haritha:2023:HBO

[HS23] Mambatta Haritha and Cherumuttathu H. Suresh. Hydrogen bonds of OC–NH motif in rings in drugs: a molecular electrostatic potential analysis. *Journal of Computational Chemistry*, 44(17):1550–1559, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hokmi:2021:CSN

[HSG21] Samaneh Hokmi, Sadegh Salehzadeh, and Yasin Gholiee. The comparison of structure, nature of bond, and electronic transitions in $[M(\eta^5\text{-Cp})(\eta^5\text{-C}_{60}Me_5)]$ ($M = Fe^{2+}$, Ru^{2+}, Os^{2+}) hybrids and corresponding metallocenes; a theoretical study. *Journal of Computational Chemistry*, 42(19):1354–1363, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Higo:2021:GEM

[HTFY21] Junichi Higo, Hajime Takashima, Yoshifumi Fukunishi, and Atsushi Yoshimori. Generalized-ensemble method study: A helix-mimetic compound inhibits protein–protein interaction by long-range and short-range intermolecular interactions. *Journal of Computational Chemistry*, 42(14):956–969, May 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hasebe:2023:TOD

[HTTT23] Masatoshi Hasebe, Takuro Tsutsumi, Tetsuya Taketsugu, and Takao Tsuneda. Total and orbital density-based analyses of molecules revealing long-range interaction regions. *Journal of Computational Chemistry*, 44(31):2391–2403, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hayashi:2023:PAD

[HUUO23] Sota Hayashi, Naoki Uemura, Masayuki Uranagase, and Shuji Ogata. Pressure-assisted decomposition of tricresyl phosphate on amorphous FeO using hybrid quantum-classical simulations. *Journal of Computational Chemistry*, 44(6):766–776, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hussain:2020:IBT

[HYA$^+$20] Razak Hussain, Rolly Yadav, Mushtaq Ahmed, Tabreiz A. Khan, Devesh Kumar, and Yusuf Akhter. Interplay between two spin states determines the hydroxylation catalyzed by P_{450} monooxygenase from *Trichoderma brevicompactum*. *Journal of Computational Chemistry*, 41(14):1330–1336, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Hou:2020:RAS

[HZG$^+$20] Chaofeng Hou, Chenglong Zhang, Wei Ge, Lei Wang, Lin Han, and Jianmin Pang. Record atomistic simulation of crystalline silicon: Bridging microscale structures and macroscale properties. *Journal of Computational Chemistry*, 41(7):731–738, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ibrahim:2024:MAH

[IAF+24] Mohammad Taha I. Ibrahim, Dunia Alatoom, Tibor Furtenbacher, Attila G. Császár, Sergei N. Yurchenko, Ala'a A. A. Azzam, and Jonathan Tennyson. MARVEL analysis of high-resolution rovibrational spectra of C O. *Journal of Computational Chemistry*, 45(13):969–984, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishak:2024:ESC

[IAS+24] Mohamad Adil Iman Ishak, Tan Tiek Aun, Nadiah Sidek, Sharifah Mohamad, Khairulazhar Jumbri, and Ninie Suhana Abdul Manan. An enantioselective study of β-cyclodextrin and ionic liquid-β-cyclodextrin towards propranolol enantiomers by molecular dynamic simulations. *Journal of Computational Chemistry*, 45(16):1329–1351, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Im:2020:CBR

[IBL20] Wonpil Im, Nilesh Banavali, and Yun Lyna Luo. Celebrating Benoît Roux's 60th birthday: quantifying biology at the membrane. *Journal of Computational Chemistry*, 41(5):385–386, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Iuchi:2021:MEH

[IK21] Satoru Iuchi and Nobuaki Koga. A model electronic Hamiltonian to describe low-lying *d–d* and metal-to-ligand charge-transfer excited states of $[Fe(bpy)_3]^{2+}$. *Journal of Computational Chemistry*, 42(3):166–179, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ivanov:2024:DBC

[IL24] Mikhail Ivanov and Alexander P. Lyubartsev. Development of a bottom-up coarse-grained model for interactions of lipids with TiO nanoparticles. *Journal of Computational Chemistry*, 45(16):1364–1379, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ishioka:2021:UGP

[IMT+21] Sora Ishioka, Itsuki Miyazato, Lauren Takahashi, Thanh Nhat Nguyen, Toshiaki Taniike, and Keisuke Takahashi. Unveiling gas-phase oxidative coupling of methane via data analysis.

Journal of Computational Chemistry, 42(20):1447–1451, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inoue:2023:AQM

[IN23a] Nobuki Inoue and Takahito Nakajima. Analytical quadrature method using recurrence formulas for two-electron integrals of frequency-dependent Breit interaction. *Journal of Computational Chemistry*, 44(26):2073–2085, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inoue:2023:RNC

[IN23b] Nobuki Inoue and Takahito Nakajima. Realistic nuclear charge distribution model function for analytic nuclear attraction integrals in Gaussian basis functions. *Journal of Computational Chemistry*, 44(11):1148–1157, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Izsak:2023:QCP

[IRB+23] Róbert Izsák, Christoph Riplinger, Nick S. Blunt, Bernardo de Souza, Nicole Holzmann, Ophelia Crawford, Joan Camps, Frank Neese, and Patrick Schopf. Quantum computing in pharma: a multilayer embedding approach for near future applications. *Journal of Computational Chemistry*, 44(3):406–421, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ignatchenko:2023:SPS

[IW23] Alexey V. Ignatchenko and Jacob P. Willower. Schwarz P-surface via isolated sp^2 carbon heptagons: Design and properties. *Journal of Computational Chemistry*, 44(9):954–961, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Irimia:2024:SCF

[IW24] Marinela Irimia and Jian Wang. Self-consistent field method for open-shell systems within the density-matrix functional theory. *Journal of Computational Chemistry*, 45(4):222–229, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inoue:2024:GFW

[IWN24] Nobuki Inoue, Yoshihiro Watanabe, and Haruyuki Nakano. Generalized Foldy–Wouthuysen transformation for relativistic two-component methods: Systematic analysis of two-component Hamiltonians. *Journal of Computational Chemistry*, 45(9):523–535, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Inamori:2020:SFA

[IYI+20] Mayu Inamori, Takeshi Yoshikawa, Yasuhiro Ikabata, Yoshifumi Nishimura, and Hiromi Nakai. Spin-flip approach within time-dependent density functional tight-binding method: Theory and applications. *Journal of Computational Chemistry*, 41(16):1538–1548, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2022:EEC

[Jab22a] Mirosław Jabłoński. Endo- and exohedral complexes of superphane with cations. *Journal of Computational Chemistry*, 43(16):1120–1133, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2022:PNU

[Jab22b] Mirosław Jabłoński. The physical nature of the ultrashort spike-ring interaction in iron maiden molecules. *Journal of Computational Chemistry*, 43(18):1206–1220, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jendoubi:2024:DMS

[JAP+24] Abir Jendoubi, Youssef Arfaoui, Jérôme Palaudoux, Muneerah Mogren Al-Mogren, and Majdi Hochlaf. DFT mechanistic study of the chemical fixation of CO_2 by aziridine derivatives. *Journal of Computational Chemistry*, 45(9):563–573, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jana:2020:ESB

[JC20] Gourhari Jana and Pratim K. Chattaraj. Effect of substitution on the bonding in He dimer confined within dodecahedrane: a computational study. *Journal of Computational Chemistry*, 41

(28):2398–2405, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jara-Cortes:2022:FAE

[JCMHT22] Jesús Jara-Cortés, Chérif F. Matta, and Jesús Hernández-Trujillo. A fast approximate extension of the interacting quantum atoms energy decomposition to excited states. *Journal of Computational Chemistry*, 43(16):1068–1078, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2020:MSU

[JFZ+20] Dandan Jiang, Mingxing Fu, Yajun Zhang, Qianqian Li, Kai Guo, Yanhui Yang, and Lili Zhao. Mechanistic study of unprecedented highly regioselective hydrocyanation of terminal alkynes: Insight into the origins of the regioselectivity and ligand effects. *Journal of Computational Chemistry*, 41(4):279–289, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Borges:2023:CAC

[JGdC+23] Itamar Borges Jr, Roberta M. P. O. Guimarães, Gabriel Monteiro de Castro, Nathália M. P. Rosa, Reed Nieman, Hans Lischka, and Adelia J. A. Aquino. A comprehensive analysis of charge transfer effects on donor-pyrene (bridge)-acceptor systems using different substituents. *Journal of Computational Chemistry*, 44(31):2424–2436, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jimenez-Gravalos:2021:CEH

[JGGPN21] Fernando Jiménez-Grávalos, Miguel Gallegos, Ángel Martín Pendás, and Alexander S. Novikov. Challenging the electrostatic σ-hole picture of halogen bonding using minimal models and the interacting quantum atoms approach. *Journal of Computational Chemistry*, 42(10):676–687, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2022:CRD

[JGK+22] Runxuan Jiang, Tarun Gogineni, Joshua Kammeraad, Yifei He, Ambuj Tewari, and Paul M. Zimmerman. Conformer-RL: a deep reinforcement learning library for conformer generation. *Journal of Computational Chemistry*, 43(27):1880–1886, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2021:FEC

[JGM21] Xiangyu Jia, Hu Ge, and Ye Mei. Free energy change estimation: The divide and conquer MBAR method. *Journal of Computational Chemistry*, 42(17):1204–1211, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jain:2022:AMA

[JGSA22] Mitisha Jain, Uwe Gerstmann, Wolf Gero Schmidt, and Hazem Aldahhak. Adatom mediated adsorption of N-heterocyclic carbenes on Cu(111) and Au(111). *Journal of Computational Chemistry*, 43(6):413–420, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jablonski:2021:DSE

[JK21] Mirosław Jabłoński and Tadeusz M. Krygowski. Dependence of the substituent energy on the level of theory. *Journal of Computational Chemistry*, 42(29):2079–2088, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2021:NPC

[JKK+21] Jaewoon Jung, Chigusa Kobayashi, Kento Kasahara, Cheng Tan, Akiyoshi Kuroda, Kazuo Minami, Shigeru Ishiduki, Tatsuo Nishiki, Hikaru Inoue, Yutaka Ishikawa, Michael Feig, and Yuji Sugita. New parallel computing algorithm of molecular dynamics for extremely huge scale biological systems. *Journal of Computational Chemistry*, 42(4):231–241, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jung:2023:AGR

[JKS23] Jaewoon Jung, Chigusa Kobayashi, and Yuji Sugita. Acceleration of generalized replica exchange with solute tempering simulations of large biological systems on massively parallel supercomputer. *Journal of Computational Chemistry*, 44(20): 1740–1749, July 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jiang:2020:TAK

[JMK+20] Tianlong Jiang, Kenta Moriwaki, Osamu Kobayashi, Kazuya Ishimura, Sebastian O. Danielache, and Shinkoh Nanbu. Theoretical analysis of the kinetic isotope effect on carboxylation in RubisCO. *Journal of Computational Chemistry*, 41(11): 1116–1123, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jharapla:2021:CDS

[JMV21] Prathap Kumar Jharapla, Subrata Mondal, and Ganapathy Vaitheeswaran. Comparative DFT study of vibrational, electronic, and optical properties of energetic alkali metal salts based on nitrogen-rich 5-aminotetrazole. *Journal of Computational Chemistry*, 42(3):180–191, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Joseph:2020:MDA

[JRS20] Newlyn N. Joseph, Raktim N. Roy, and Thomas A. Steitz. Molecular dynamics analysis of Mg^{2+}-dependent cleavage of a pistol ribozyme reveals a fail-safe secondary ion for catalysis. *Journal of Computational Chemistry*, 41(14):1345–1352, May 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jager:2021:VOP

[JS21] Marc Jäger and Rolf Schäfer. Variation of the optical properties with size and composition of small, isolated $Cd_xSe_y^+$ clusters. *Journal of Computational Chemistry*, 42(5):303–309, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Jia:2024:HMC

[JWS+24] Lifan Jia, Yunxia Wang, Lulu Song, Ruirui Liu, Longgang Li, Jisheng Li, Yongquan Zhou, Jianmin Pan, and Fayan Zhu. Hydrolysis mechanism of the cyclohexaborate anion: Unraveling the intricacies. *Journal of Computational Chemistry*, 45(17): 1456–1469, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Dunning:2024:ESL

[JX24] Thom H. Dunning Jr and Lu T. Xu. Electronic structure of $Li_{1,2,3}^{+,0,-}$ and nature of the bonding in $Li_{2,3}^{+,0,-}$. *Journal of Com-*

putational Chemistry, 45(7):405–418, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kong:2022:MPR

[KB22] Linghan Kong and Richard A. Bryce. Modeling pyranose ring pucker in carbohydrates using machine learning and semi-empirical quantum chemical methods. *Journal of Computational Chemistry*, 43(30):2009–2022, November 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kohn:2023:CSG

[KBHG23] Julia Kohn, Markus Bursch, Andreas Hansen, and Stefan Grimme. Computational study of ground-state properties of μ_2-bridged group 14 porphyrinic sandwich complexes. *Journal of Computational Chemistry*, 44(3):229–239, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kuzela:2024:SAE

[KBK+24] Tomás Kuzela, Dmitrij Bondarev, Eva Kutálková, Zuzana Benková, Josef Hrncirík, and Marek Ingr. Study of absorption and emission spectra of substituted terthiophene compounds by methods of theoretical chemistry. *Journal of Computational Chemistry*, 45(16):1404–1418, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khelashvili:2020:MLB

[KCF+20] George Khelashvili, Xiaolu Cheng, Maria E. Falzone, Milka Doktorova, Alessio Accardi, and Harel Weinstein. Membrane lipids are both the substrates and a mechanistically responsive environment of TMEM16 scramblase proteins. *Journal of Computational Chemistry*, 41(6):538–551, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaiser:2020:MCS

[KCGK20] Jan Kaiser, Mike Castellano, David Gnandt, and Thorsten Koslowski. Monte Carlo simulation and thermodynamic integration applied to protein charge transfer. *Journal of Computational Chemistry*, 41(11):1105–1115, April 30, 2020. CO-

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

Khatri:2021:FPB

[KDKS21] Vikas Khatri, Harender S. Dhattarwal, Hemant K. Kashyap, and Gurmeet Singh. First-principles based theoretical investigation of impact of polyolefin structure on photooxidation behavior. *Journal of Computational Chemistry*, 42(24):1710–1719, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Korsaye:2022:FDE

[KdlLC22] Feven Alemu Korsaye, Aurélien de la Lande, and Ilaria Ciofini. Following the density evolution using real time density functional theory and density based indexes: Application to model push-pull molecules. *Journal of Computational Chemistry*, 43 (22):1464–1473, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kiani:2021:MLE

[KDLP21] Pirouz Kiani, Elaine S. Dodsworth, A. B. P. Lever, and William J. Pietro. Modeling ligand electrochemical parameters by repulsion-corrected eigenvalues. *Journal of Computational Chemistry*, 42(17):1236–1242, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karnamkkott:2024:SMA

[KDMM24] Harsha S. Karnamkkott, Sujit Das, Totan Mondal, and Kartik Chandra Mondal. Small molecule activation by sila/germa boryne species. *Journal of Computational Chemistry*, 45(11): 804–819, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2022:PML

[KDP+22] Sivakumar Prasanth Kumar, Nandan Y. Dixit, Chirag N. Patel, Rakesh M. Rawal, and Himanshu A. Pandya. PharmRF: a machine-learning scoring function to identify the best protein-ligand complexes for structure-based pharmacophore screening with high enrichments. *Journal of Computational Chemistry*, 43(12):847–863, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karachi:2023:BC

[KE23a] Sara Sadat Karachi and Kiamars Eskandari. Back cover. *Journal of Computational Chemistry*, 44(9):C4, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karachi:2023:BHS

[KE23b] Sara Sadat Karachi and Kiamars Eskandari. Bonding in the high spin lithium clusters: Non-nuclear attractors play a crucial role. *Journal of Computational Chemistry*, 44(9):962–968, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krog:2023:MCA

[KEK23] Dan Krog, Martin B. Enghoff, and Christoph Köhn. A Monte Carlo approach to study the effect of ions on the nucleation of sulfuric acid-water clusters. *Journal of Computational Chemistry*, 44(13):1250–1262, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klemm:2024:MLA

[KF24] Carl Philipp Klemm and Till Frömling. Machine learning assisted analysis of equivalent circuit usage in electrochemical impedance spectroscopy applications. *Journal of Computational Chemistry*, 45(16):1380–1389, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klein:2021:NIC

[KFLP21] Johanna Klein, Paul Fleurat-Lessard, and Julien Pilmé. New insights in chemical reactivity from quantum chemical topology. *Journal of Computational Chemistry*, 42(12):840–854, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klaja:2020:CI

[KFTB20a] Oskar Klaja, James A. Frank, Dirk Trauner, and Ana-Nicoleta Bondar. Cover image. *Journal of Computational Chemistry*, 41(27):C1, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Klaja:2020:PEF

[KFTB20b] Oskar Klaja, James A. Frank, Dirk Trauner, and Ana-Nicoleta Bondar. Potential energy function for a photo-switchable lipid molecule. *Journal of Computational Chemistry*, 41(27):2336–2351, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khire:2023:DTA

[KG23] Subodh S. Khire and Shridhar R. Gadre. Development and testing of an algorithm for efficient MP2/CCSD(T) energy estimation of molecular clusters with the 2-body approach. *Journal of Computational Chemistry*, 44(3):261–267, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kwapien:2021:IIE

[KGD+21] Karolina Kwapien, Laurent Gavara, Jean-Denis Docquier, Dorothée Berthomieu, Jean-François Hernandez, and Nohad Gresh. Intermolecular interactions of the extended recognition site of VIM-2 metallo-β-lactamase with 1,2,4-triazole-3-thione inhibitors. Validations of a polarizable molecular mechanics potential by ab initio QC. *Journal of Computational Chemistry*, 42(2):86–106, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khajehpasha:2021:NST

[KGG21] Ehsan Rahmatizad Khajehpasha, Stefan Goedecker, and S. Alireza Ghasemi. New strontium titanate polymorphs under high pressure. *Journal of Computational Chemistry*, 42 (10):699–705, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kar:2021:AFA

[KGS+21] Moumita Kar, Atish Ghosh, Ritabrata Sarkar, Sougata Pal, and Pranab Sarkar. Arene and functionalized arene based two dimensional organic-inorganic hybrid perovskites for photovoltaic applications. *Journal of Computational Chemistry*, 42 (27):1982–1990, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Katsyuba:2022:CAS

[KGS+22] Sergey A. Katsyuba, Tatiana P. Gerasimova, Sebastian Spicher, Fabian Bohle, and Stefan Grimme. Computer-aided simulation of infrared spectra of ethanol conformations in gas, liquid and in CCl_4 solution. *Journal of Computational Chemistry*, 43(4):279–288, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kogut:2021:PCG

[KGTL21] Mateusz Kogut, Zhou Gong, Chun Tang, and Adam Liwo. Pseudopotentials for coarse-grained cross-link-assisted modeling of protein structures. *Journal of Computational Chemistry*, 42(29):2054–2067, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirboga:2024:EAI

[KI24] Kevser Kübra Kirboga and Mesut Isik. Explainable artificial intelligence in the design of selective carbonic anhydrase I–II inhibitors via molecular fingerprinting. *Journal of Computational Chemistry*, 45(18):1530–1539, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirkland:2023:CIF

[KJV23] Justin K. Kirkland, Sophia K. Johnson, and Konstantinos D. Vogiatzis. Computational investigation of functionalized carbenes on dinitrogen activation. *Journal of Computational Chemistry*, 44(7):832–842, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kraus:2022:TIG

[KK22a] Jakob Kraus and Jens Kortus. A theoretical investigation into gallic acid pyrolysis. *Journal of Computational Chemistry*, 43 (15):1023–1032, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kroeger:2022:CI

[KK22b] Asja A. Kroeger and Amir Karton. Cover image. *Journal of Computational Chemistry*, 43(2):i, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kroeger:2022:GIP

[KK22c] Asja A. Kroeger and Amir Karton. Graphene-induced planarization of cyclooctatetraene derivatives. *Journal of Computational Chemistry*, 43(2):96–105, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kido:2023:CHL

[KK23] Kentaro Kido and Masashi Kaneko. Conformation, hydration, and ligand exchange process of ruthenium nitrosyl complexes in aqueous solution: Free-energy calculations by a combination of molecular-orbital theories and different solvent models. *Journal of Computational Chemistry*, 44(4):546–558, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kotaru:2023:MEI

[KKAK23] Saikiran Kotaru, Sven Kähler, Maristella Alessio, and Anna I. Krylov. Magnetic exchange interactions in binuclear and tetranuclear iron(III) complexes described by spin-flip DFT and Heisenberg effective Hamiltonians. *Journal of Computational Chemistry*, 44(3):367–380, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kasper:2020:NTO

[KL20] Joseph M. Kasper and Xiaosong Li. Natural transition orbitals for complex two-component excited state calculations. *Journal of Computational Chemistry*, 41(16):1557–1563, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khelifi:2024:PAM

[KLC+24] Roumaissa Khelifi, Nadjia Latelli, Zoulikha Charifi, Christophe Morell, and Henry Chermette. Predicting the activity of methoxyphenol derivatives antioxidants: II-Importance of the nature of the solvent on the mechanism, a DFT study. *Journal of Computational Chemistry*, 45(12):886–897, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kloo:2022:CSI

[Klo22] Lars Kloo. On closed-shell interactions between heavy main-group elements. *Journal of Computational Chemistry*, 43(29):

1985–1996, November 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kognole:2022:PCG

[KLP+22] Abhishek A. Kognole, Jumin Lee, Sang-Jun Park, Sunhwan Jo, Payal Chatterjee, Justin A. Lemkul, Jing Huang, Alexander D. MacKerell, Jr., and Wonpil Im. CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. *Journal of Computational Chemistry*, 43(5):359–375, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2023:BHA

[KLZ+23] Seonghan Kim, Yi Liu, Matthew Ziarnik, Sangjae Seo, Yiwei Cao, X. Frank Zhang, and Wonpil Im. Binding of human ACE2 and RBD of omicron enhanced by unique interaction patterns among SARS-CoV-2 variants of concern. *Journal of Computational Chemistry*, 44(4):594–601, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kanamaru:2022:FAE

[KM22] Yuki Kanamaru and Toru Matsui. Factor analysis of error in oxidation potential calculation: a machine learning study. *Journal of Computational Chemistry*, 43(22):1504–1512, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2024:TSB

[KM24] Hyunsik Kim and Jorge A. Morales. Testing standard basis sets for direct ionizations: $H^+ + H$ at $E_{\mathrm{Lab}} = 0.1$–100 keV. *Journal of Computational Chemistry*, 45(10):671–682, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khan:2024:CIP

[KMR+24] Muhammad Sanwal Khan, Nasir Maha, Maira Riaz, Tahira Yasmin, Ahmad Irfan, and Muhammad Asim Raza Basra. Computational investigation of pyrazinamide drugs and its transition metal complexes using a DFT approach. *Journal of Computational Chemistry*, 45(10):622–632, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kapakayala:2021:BCS

[KN21] Anji Babu Kapakayala and Nisanth N. Nair. Boosting the conformational sampling by combining replica exchange with solute tempering and well-sliced metadynamics. *Journal of Computational Chemistry*, 42(31):2233–2240, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koehl:2021:PEN

[KOD21] Patrice Koehl, Henri Orland, and Marc Delarue. Parameterizing elastic network models to capture the dynamics of proteins. *Journal of Computational Chemistry*, 42(23):1643–1661, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2022:ICA

[Kop22a] Jacek Koput. Ab initio characterization of the aluminum dimer in its $X^3\Pi_u$ and A $^3\Sigma_g^-$ electronic states. *Journal of Computational Chemistry*, 43(14):986–993, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koput:2022:GSP

[Kop22b] Jacek Koput. Ground-state potential energy functions and vibration-rotation energy levels of beryllium lithium and its cation. *Journal of Computational Chemistry*, 43(7):491–498, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kosenkov:2022:PSE

[Kos22] Dmitri Kosenkov. `PyFREC 2.0`: Software for excitation energy transfer modeling. *Journal of Computational Chemistry*, 43(19):1320–1328, July 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirschbaum:2022:EOA

[KPDB22] Thorren Kirschbaum, Tristan Petit, Joachim Dzubiella, and Annika Bande. Effects of oxidative adsorbates and cluster formation on the electronic structure of nanodiamonds. *Journal of Computational Chemistry*, 43(13):923–929, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kramer:2023:ESD

[KPHV23] Aaron Kramer, Ruth Pachter, Julia W. P. Hsu, and William G. Vandenberghe. The effect of solvent on determining highest occupied molecular orbital energies of semiconducting organic molecules: Insight from a combined computational approach. *Journal of Computational Chemistry*, 44(10):1064–1072, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2023:BPS

[KPKS23] Yenamareddy Bhargav Kumar, Anwesh Pandey, Nandan Kumar, and G. Narahari Sastry. Binding propensity and selectivity of cationic, anionic, and neutral guests with model hydrophobic hosts: a first principles study. *Journal of Computational Chemistry*, 44(3):432–441, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koliogiorgos:2023:ETB

[KPR23] Athanasios Koliogiorgos, Tomas Polcar, and Bohuslav Rezek. Energy transfer between Si nanocrystals and protoporphyrin molecules as a function of distance, orientation and size. *Journal of Computational Chemistry*, 44(11):1138–1147, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karpov:2021:HSM

[KPTT21] Valerii V. Karpov, Aleksandra M. Puzyk, Peter M. Tolstoy, and Elena Yu. Tupikina. Hydration of selenolate moiety: Ab initio investigation of properties of O-H$\cdots$Se(-) hydrogen bonds in $CH_3Se(-)\cdots(H_2O)_n$ clusters. *Journal of Computational Chemistry*, 42(28):2014–2023, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalathingal:2023:MMB

[KR23] Mahroof Kalathingal and Young Min Rhee. Molecular mechanism of binding between a therapeutic RNA aptamer and its protein target VEGF: a molecular dynamics study. *Journal of Computational Chemistry*, 44(11):1129–1137, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kim:2023:FPL

[KRSD+23] Taewon D. Kim, M. Richer, Gabriela Sánchez-Díaz, Ramón Alain Miranda-Quintana, Toon Verstraelen, Farnaz Heidar-Zadeh, and Paul W. Ayers. `Fanpy`: a Python library for prototyping multideterminant methods in *ab initio* quantum chemistry. *Journal of Computational Chemistry*, 44(5):697–709, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kalayan:2024:NNP

[KRW+24] Jas Kalayan, Ismaeel Ramzan, Christopher D. Williams, Richard A. Bryce, and Neil A. Burton. A neural network potential based on pairwise resolved atomic forces and energies. *Journal of Computational Chemistry*, 45(14):1143–1151, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Karton:2021:EDF

[KS21] Amir Karton and Peter R. Spackman. Evaluation of density functional theory for a large and diverse set of organic and inorganic equilibrium structures. *Journal of Computational Chemistry*, 42(22):1590–1601, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Krishnapriya:2024:UPB

[KS24] Vilakkathala U. Krishnapriya and Cherumuttathu H. Suresh. Unraveling pnicogen bonding cooperativity: Insights from molecular electrostatic potential analysis. *Journal of Computational Chemistry*, 45(8):461–475, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Konovalov:2021:MBN

[KSP21] Anton Konovalov, Benjamin C. B. Symons, and Paul L. A. Popelier. On the many-body nature of intramolecular forces in FFLUX and its implications. *Journal of Computational Chemistry*, 42(2):107–116, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:2021:RMT

[KSRB+21] Tomomi Kondo, Takehiko Sasaki, Sergi Ruiz-Barragan, Jordi Ribas-Ariño, and Motoyuki Shiga. Refined metadynamics through canonical sampling using time-invariant bias potential: a study of polyalcohol dehydration in hot acidic solutions. *Journal of Computational Chemistry*, 42(3):156–165, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kotowski:2021:PEA

[KSRKS21] Krzysztof Kotowski, Tomasz Smolarczyk, Irena Roterman-Konieczna, and Katarzyna Stapor. ProteinUnet — an efficient alternative to SPIDER3-single for sequence-based prediction of protein secondary structures. *Journal of Computational Chemistry*, 42(1):50–59, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:2021:CI

[KSS21a] Tomomi Kondo, Takehiko Sasaki, and Motoyuki Shiga. Cover image. *Journal of Computational Chemistry*, 42(25):i, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kondo:2021:MSD

[KSS21b] Tomomi Kondo, Takehiko Sasaki, and Motoyuki Shiga. The mechanism of sorbitol dehydration in hot acidic solutions. *Journal of Computational Chemistry*, 42(25):1783–1791, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kour:2023:DMC

[KTBS23] Manjinder Kour, Attila Taborosi, Eric S. Boyd, and Robert K. Szilagyi. Development of molecular cluster models to probe pyrite surface reactivity. *Journal of Computational Chemistry*, 44(32):2486–2500, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kurisaki:2023:TCC

[KTM+23] Ikuo Kurisaki, Seiya Tanaka, Ichiro Mori, Toshihito Umegaki, Yoshiharu Mori, and Shigenori Tanaka. Thermal conductivity and conductance of protein in aqueous solution: Effects of geometrical shape. *Journal of Computational Chemistry*, 44 (7):857–868, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kusumoto:2020:SIA

[KUNT20] Miyu Kusumoto, Kaori Ueno-Noto, and Keiko Takano. Systematic interaction analysis of anti-human immunodeficiency virus Type-1 neutralizing antibodies with high mannose glycans using fragment molecular orbital and molecular dynamics methods. *Journal of Computational Chemistry*, 41(1):31–42, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kaur:2022:LSH

[KW22] Aishvaryadeep Kaur and David J. D. Wilson. Ligand-stabilized heteronuclear diatomics of group 13 and 15. *Journal of Computational Chemistry*, 43(29):1964–1977, November 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kirschbaum:2024:GES

[KWB24] Thorren Kirschbaum, Xiangfei Wang, and Annika Bande. Ground and excited state charge transfer at aqueous nanodiamonds. *Journal of Computational Chemistry*, 45(11):710–718, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koots:2024:FC

[KWMPR24a] Rian Koots, Yu Wang, Marjan Mirahmadi, and Jesús Pérez-Ríos. Front cover. *Journal of Computational Chemistry*, 45 (17):C1, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Koots:2024:PSC

[KWMPR24b] Rian Koots, Yu Wang, Marjan Mirahmadi, and Jesús Pérez-Ríos. `Py3BR`: [a] software for computing atomic three-body recombination rates. *Journal of Computational Chemistry*, 45(17):1505–1514, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ke:2023:CCN

[KWX23] Zhipeng Ke, Jingwei Weng, and Xin Xu. Calculating ^{13}C NMR chemical shifts of large molecules using the eXtended ONIOM method at high accuracy with a low cost. *Journal of Computational Chemistry*, 44(30):2347–2357, November 15,

2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kanemaru:2023:SEF

[KWYN23] Kodai Kanemaru, Yoshihiro Watanabe, Norio Yoshida, and Haruyuki Nakano. Solvent effects in four-component relativistic electronic structure theory based on the reference interaction-site model. *Journal of Computational Chemistry*, 44(1):5–14, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kumar:2020:FSP

[KYM20] Anmol Kumar, Ozge Yoluk, and Alexander D. MacKerell Jr. FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules. *Journal of Computational Chemistry*, 41(9):958–970, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Korotenko:2024:SOC

[KZ24] Vasilii Korotenko and Hendrik Zipse. The stability of oxygen-centered radicals and its response to hydrogen bonding interactions. *Journal of Computational Chemistry*, 45(2):101–114, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kacka-Zych:2021:UMM

[KZJ21] Agnieszka Kacka-Zych and Radomir Jasiński. Understanding the molecular mechanism of γ-elimination of nitrous acid in the framework of the molecular electron density theory. *Journal of Computational Chemistry*, 42(17):1195–1203, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kacka-Zych:2022:MAS

[KZJ22] Agnieszka Kacka-Zych and Radomir Jasiński. Mechanistic aspects of the synthesis of seven-membered internal nitronates via stepwise [4 + 3] cycloaddition involving conjugated nitroalkenes: Molecular Electron Density Theory computational study. *Journal of Computational Chemistry*, 43(18):1221–1228, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Kelich:2023:BPS

[KZOV23] Payam Kelich, Huanhuan Zhao, Jose R. Orona, and Lela Vuković. `BinderSpace`: a package for sequence space analyses for datasets of affinity-selected oligonucleotides and peptide-based molecules. *Journal of Computational Chemistry*, 44(22): 1836–1844, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Khakimov:2022:TTC

[KZP22] Dmitry V. Khakimov, Victor P. Zelenov, and Tatyana S. Pivina. Di- and trioxides of triazolotetrazine: Computational prediction of crystal structures and estimation of physicochemical characteristics. *Journal of Computational Chemistry*, 43(11): 778–784, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lev:2020:SIC

[LA20] Bogdan Lev and Toby W. Allen. Simulating ion channel activation mechanisms using swarms of trajectories. *Journal of Computational Chemistry*, 41(5):387–401, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2023:SMW

[LAM+23] Hui Lu, Alireza Azizi, Xiao Peng Mi, Yu Wenjing, Yutting Peng, Tianlv Xu, Herbert Früchtl, Tanja van Mourik, Steven R. Kirk, and Samantha Jenkins. Scoring molecular wires subject to an ultrafast laser pulse for molecular electronic devices. *Journal of Computational Chemistry*, 44(21): 1776–1785, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laun:2021:BCC

[LB21] Joachim Laun and Thomas Bredow. BSSE-corrected consistent Gaussian basis sets of triple-zeta valence with polarization quality of the sixth period for solid-state calculations. *Journal of Computational Chemistry*, 42(15):1064–1072, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laun:2022:BCC

[LB22] Joachim Laun and Thomas Bredow. BSSE-corrected consistent Gaussian basis sets of triple-zeta valence with polarization quality of the fifth period for solid-state calculations. *Journal of Computational Chemistry*, 43(12):839–846, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Long:2022:ERP

[LBH+22] Danny K. Long, Wolfgang Bangerth, Derek R. Handwerk, Christopher B. Whitehead, Patrick D. Shipman, and Richard G. Finke. Estimating reaction parameters in mechanism-enabled population balance models of nanoparticle size distributions: a Bayesian inverse problem approach. *Journal of Computational Chemistry*, 43(1):43–56, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2022:IGM

[LC22] Tian Lu and Qinxue Chen. Independent gradient model based on Hirshfeld partition: a new method for visual study of interactions in chemical systems. *Journal of Computational Chemistry*, 43(8):539–555, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laplaza:2021:OEN

[LCC+21] Rubén Laplaza, Carlos Cárdenas, Patrick Chaquin, Julia Contreras-García, and Paul W. Ayers. Orbital energies and nuclear forces in DFT: Interpretation and validation. *Journal of Computational Chemistry*, 42(5):334–343, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liza:2024:ISC

[LCLB24] Nishattasnim Liza, Daniel J. Coe, Yuhui Lu, and Enrique P. Blair. *Ab initio* studies of counterion effects in molecular quantum-dot cellular automata. *Journal of Computational Chemistry*, 45(7):392–404, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez-Carballeira:2021:NPI

[LCP21] Diego López-Carballeira and Tomás Polcar. A new protocol for the identification of singlet fission sensitizers through computational screening. *Journal of Computational Chemistry*, 42 (31):2241–2249, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez-Carballeira:2024:HTS

[LCP24] Diego López-Carballeira and Tomás Polcar. High throughput selection of organic cathode materials. *Journal of Computational Chemistry*, 45(5):264–273, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luise:2022:MSP

[LDT+22] Davide Luise, Massimo Christian D'Alterio, Giovanni Talarico, Ilaria Ciofini, and Frédéric Labat. Modeling the spectral properties of poly(x-phenylenediamine) conducting polymers using a combined TD-DFT and electrostatic embedding approach. *Journal of Computational Chemistry*, 43(30):2001–2008, November 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lourenco:2021:MDS

[LEP+21] Tuanan C. Lourenço, Mahsa Ebadi, Matthew J. Panzer, Daniel Brandell, and Luciano T. Costa. A molecular dynamics study of a fully zwitterionic copolymer/ionic liquid-based electrolyte: Li^+ transport mechanisms and ionic interactions. *Journal of Computational Chemistry*, 42(23):1689–1703, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2021:AAS

[LGC21] Xiaorong Liu, Xiping Gong, and Jianhan Chen. Accelerating atomistic simulations of proteins using multiscale enhanced sampling with independent tempering. *Journal of Computational Chemistry*, 42(5):358–364, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lian:2020:AMD

[LGD+20] Peng Lian, Luanjing Guo, Deepa Devarajan, Jerry M. Parks, Scott L. Painter, Scott C. Brooks, and Jeremy C. Smith. The AQUA-MER databases and aqueous speciation server: a web resource for multiscale modeling of mercury speciation. *Journal of Computational Chemistry*, 41(2):147–155, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lamine:2022:TER

[LGJF22] Walid Lamine, Frédéric Guégan, François Jérôme, and Gilles Frapper. Theoretical exploration of the reactivity of cellulose models under non-thermal plasma conditions-mechanistic and NBO studies. *Journal of Computational Chemistry*, 43(20): 1334–1341, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lefrancois-Gagnon:2020:TUS

[LGM20] Kevin M. Lefrançois-Gagnon and Robert C. Mawhinney. Toward universal substituent constants: Model chemistry sensitivity of descriptors from the quantum theory of atoms in molecules. *Journal of Computational Chemistry*, 41(29):2485–2503, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lefrancois-Gagnon:2022:TUS

[LGM22] Kevin M. Lefrancois-Gagnon and Robert C. Mawhinney. Toward universal substituent constants: Transferability of group descriptors from the quantum theory of atoms in molecules. *Journal of Computational Chemistry*, 43(4):265–278, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lourenco:2024:RLS

[LHB$^+$24] Maicon Pierre Lourenço, Jirí Hostas, Colin Bellinger, Alain Tchagang, and Dennis R. Salahub. Reinforcement learning for in silico determination of adsorbate-substrate structures. *Journal of Computational Chemistry*, 45(15):1289–1302, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2021:TNS

[LHC$^+$21] Feng Li, Weibo Han, Zhi Cao, Shilei Ji, Haiyun Wang, Lixia Wang, Hong Wu, Yuping Zhu, and Yong Pu. Two novel semiconducting b_2 CO monolayers with high carrier mobilities. *Journal of Computational Chemistry*, 42(28):2024–2030, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luy:2023:BCI

[LHG+23] Jan-Niclas Luy, Pascal Henkel, Daniel Grigjanis, Jannis Jung, Doreen Mollenhauer, and Ralf Tonner-Zech. Bonding character of intermediates in on-surface Ullmann reactions revealed with energy decomposition analysis. *Journal of Computational Chemistry*, 44(3):179–189, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2021:PPB

[LHH+21] In Seong Lee, Jong-Kwon Ha, Daeho Han, Tae In Kim, Sung Wook Moon, and Seung Kyu Min. PyUNIxMD: a Python-based excited state molecular dynamics package. *Journal of Computational Chemistry*, 42(24):1755–1766, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lourenco:2023:GGA

[LHH+23] Maicon Pierre Lourenço, Jirí Hostas, Lizandra Barrios Herrera, Patrizia Calaminici, Andreas M. Köster, Alain Tchagang, and Dennis R. Salahub. `GAMaterial` — a genetic-algorithm software for material design and discovery. *Journal of Computational Chemistry*, 44(7):814–823, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lin:2020:IMC

[LJ20] Fang-Yu Lin and Alexander D. MacKerell Jr. Improved modeling of cation–π and anion-ring interactions using the Drude polarizable empirical force field for proteins. *Journal of Computational Chemistry*, 41(5):439–448, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lu:2023:HOS

[LJW+23] Jun-Bo Lu, Xue-Lian Jiang, Jia-Qi Wang, Han-Shi Hu, W. H. Eugen Schwarz, and Jun Li. On the highest oxidation states of the actinoids in AnO_4 molecules (An = Ac–Cm): a DMRG-CASSCF study. *Journal of Computational Chemistry*, 44(3):190–198, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Leskourova:2022:ECH

[LK22] Aneta Leskourová and Michal H. Kolár. The effect of off-center σ-hole on the atom-centered partial charges in halogenated molecules. *Journal of Computational Chemistry*, 43(12):864–869, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Levina:2022:KET

[LKAT22] Elena O. Levina, Maria G. Khrenova, Andrey A. Astakhov, and Vladimir G. Tsirelson. Keto-enol tautomerism from the electron delocalization perspective. *Journal of Computational Chemistry*, 43(15):1000–1010, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lefebvre:2023:IPI

[LKK+23] C. Lefebvre, J. Klein, H. Khartabil, J.-C. Boisson, and E. Hénon. `IGMPlot`: a program to identify, characterize, and quantify molecular interactions. *Journal of Computational Chemistry*, 44(20):1750–1766, July 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Larsson:2020:MTC

[LKM20] Per Larsson, Rosita C. Kneiszl, and Erik G. Marklund. MkVsites: a tool for creating GROMACS virtual sites parameters to increase performance in all-atom molecular dynamics simulations. *Journal of Computational Chemistry*, 41(16): 1564–1569, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Levina:2021:ERE

[LKT21] Elena O. Levina, Maria G. Khrenova, and Vladimir G. Tsirelson. The explicit role of electron exchange in the hydrogen bonded molecular complexes. *Journal of Computational Chemistry*, 42(12):870–882, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lai:2021:NGC

[LL21a] San Kiong Lai and Chong Chiat Lim. Neutral gold clusters studied by the isothermal Brownian-type molecular dynamics and metadynamics molecular dynamics simulations. *Journal of Computational Chemistry*, 42(5):310–325, February 15,

2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lubecka:2021:EAE

[LL21b] Emilia A. Lubecka and Adam Liwo. ESCASA: Analytical estimation of atomic coordinates from coarse-grained geometry for nuclear-magnetic-resonance-assisted protein structure modeling. I. Backbone and H^{β} protons. *Journal of Computational Chemistry*, 42(22):1579–1589, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lubecka:2022:CGA

[LL22] Emilia A. Lubecka and Adam Liwo. A coarse-grained approach to NMR-data-assisted modeling of protein structures. *Journal of Computational Chemistry*, 43(31):2047–2059, December 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2024:EFM

[LLJ+24] Xunshan Liu, Zhen Liang, Zhetong Jin, Xu Zhang, and Chengshuo Shen. Enantiomerization of five-membered-heterocycle-embedded helicenes: a DFT study. *Journal of Computational Chemistry*, 45(8):454–460, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Langstieh:2023:LTD

[LLKS23] Derek R. Langstieh, Richard H. Duncan Lyngdoh, Robert Bruce King, and Henry F. Schaefer. Lantern-type dinickel complexes: an exploration of possibilities for nickel-nickel bonding with bridging bidentate ligands. *Journal of Computational Chemistry*, 44(3):355–366, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Labiak:2022:DGP

[LLS22a] Rodrigo Labiak, Carlile Lavor, and Michael Souza. Distance geometry and protein loop modeling. *Journal of Computational Chemistry*, 43(5):349–358, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2022:BCM

[LLS+22b] Xuening Li, Ying Li, Yuanyuan Sun, Lingpeng Meng, and Yanli Zeng. BF_3-catalyzed Mukaiyama aldol reaction of acetaldehyde with 2-siloxy-1-propene. *Journal of Computational Chemistry*, 43(6):402–412, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2023:SRE

[LLZ+23] Xiao-Lei Li, Chao-Ming Li, Jia-Yi Zhu, Zhan Zhou, Qiang Hao, and Chang-Sheng Wang. A scheme for rapid evaluation of the intermolecular three-body polarization effect in water clusters. *Journal of Computational Chemistry*, 44(5): 677–686, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lakra:2024:FPS

[LM24] Sangeeta Lakra and S. K. Mukherjee. First principle studies on structural, elastic, electronic, optical, and thermoelectric properties of new perovskite $TlTaO_3$: For renewable energy applications. *Journal of Computational Chemistry*, 45(13): 1008–1016, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lo:2023:USH

[LML+23] Rabindranath Lo, Anna Masínová, Maximilián Lamanec, Dana Nachtigallová, and Pavel Hobza. The unusual stability of H-bonded complexes in solvent caused by greater solvation energy of complex compared to those of isolated fragments. *Journal of Computational Chemistry*, 44(3):329–333, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luy:2021:EHM

[LMPT21] Jan-Niclas Luy, Mahlet Molla, Lisa Pecher, and Ralf Tonner. Efficient hierarchical models for reactivity of organic layers on semiconductor surfaces. *Journal of Computational Chemistry*, 42(12):827–839, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lazaric:2023:SFE

[LPF+23] Aleksandar Lazaric, Viren Pattni, Kaprao Fuegner, Arieh Ben-Naim, and Matthias Heyden. Solvation free energy arithmetic for small organic molecules. *Journal of Computational Chemistry*, 44(13):1263–1277, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Laghuvarapu:2020:BND

[LPP20] Siddhartha Laghuvarapu, Yashaswi Pathak, and U. Deva Priyakumar. BAND NN: a deep learning framework for energy prediction and geometry optimization of organic small molecules. *Journal of Computational Chemistry*, 41(8):790–799, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2020:HVH

[LR20] Jingbai Li and Andrey Yu. Rogachev. Homolytic versus heterolytic bond breaking in functionalized $[R\text{-}C_{20}H_{10}]^{+}$ systems. *Journal of Computational Chemistry*, 41(2):88–96, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2021:APP

[LRF+21] Musen Li, Jeffrey R. Reimers, Michael J. Ford, Rika Kobayashi, and Roger D. Amos. Accurate prediction of the properties of materials using the CAM-B3LYP density functional. *Journal of Computational Chemistry*, 42(21):1486–1497, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ligorio:2023:BBD

[LRKD23] Raphael F. Ligório, José L. Rodrigues, Anna Krawczuk, and Leonardo H. R. Dos Santos. A building-block database of distributed polarizabilities and dipole moments to estimate optical properties of biomacromolecules in isolation or in an explicitly solvated medium. *Journal of Computational Chemistry*, 44(6):745–754, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2022:DQM

[LRqG+22] Cui Liu, Yang Ren, Xiao qin Gao, Xue Du, and Zhong zhi Yang. Development of QM/MM (ABEEM polarizable force field) method to simulate the excision reaction mechanism of damaged cytosine. *Journal of Computational Chemistry*, 43 (32):2139–2153, December 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lipska:2023:LTS

[LSC+23] Agnieszka G. Lipska, Adam K. Sieradzan, Cezary Czaplewski, Andrea D. Lipińska, Krzysztof M. Ocetkiewicz, Jerzy Proficz, Paweł Czarnul, Henryk Krawczyk, and Adam Liwo. Long-time scale simulations of virus-like particles from three human-norovirus strains. *Journal of Computational Chemistry*, 44 (16):1470–1483, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez-Sosa:2024:CRW

[LSC24] L. López-Sosa and P. Calaminici. Cycloaddition reactions via "*on water*" protocol reactions: a density functional theory study. *Journal of Computational Chemistry*, 45(10):595–609, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lopez-Sosa:2023:CCQ

[LSCK23] L. López-Sosa, P. Calaminici, and A. M. Köster. Cartesian constraints in QM/MM optimizations. *Journal of Computational Chemistry*, 44(30):2358–2368, November 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2023:BAM

[LSP23] Seho Lee, Chaok Seok, and Hahnbeom Park. Benchmarking applicability of medium-resolution cryo-EM protein structures for structure-based drug design. *Journal of Computational Chemistry*, 44(14):1360–1368, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Levina:2023:DPC

[LT23] Elena O. Levina and Vladimir G. Tsirelson. DFT potentials from a chemical perspective: Anatomy of electron (de)localization in molecules and crystals. *Journal of Computational Chemistry*, 44(22):1817–1835, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2024:BBC

[LWC+24] Lina Liu, Zhihong Wei, Qiang Chen, Chaoren Shen, Tonghao Shen, Xinxin Tian, and Si-Dian Li. Benchmarking boron cluster calculations: Establishing reliable geometrical and energetic references for B_n (n = 1–4). *Journal of Computational Chemistry*, 45(3):159–169, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2022:SPI

[LWF+22] Yunzhi Li, Dong Wang, Fangjia Fu, Qiying Xia, Wei Li, and Shuhua Li. Structures and properties of ionic crystals and condensed phase ionic liquids predicted with the generalized energy-based fragmentation method. *Journal of Computational Chemistry*, 43(10):704–716, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Luise:2021:MUV

[LWLC21] Davide Luise, Liam Wilbraham, Frédéric Labat, and Ilaria Ciofini. Modeling UV-Vis spectra of low dimensional materials using electrostatic embedding: The case of CdSe. *Journal of Computational Chemistry*, 42(17):1212–1224, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Liu:2022:GES

[LXP+22] Dong Liu, Song Xu, Gerui Pei, Jianzhi Xu, Xintian Zhao, Chuncai Kong, Zhimao Yang, and Tao Yang. Geometries, electronic structures, and bonding properties of endohedral group-14 Zintl clusters TM@E_{10} (TM = Fe, Co, Ni; E = Ge, Sn, Pb). *Journal of Computational Chemistry*, 43(12):828–838, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Lee:2023:GHP

[LYKS23] Changsoo Lee, Jinsol Yang, Sohee Kwon, and Chaok Seok. `GalaxyDock2-HEME`: Protein-ligand docking for heme proteins. *Journal of Computational Chemistry*, 44(14):1369–1380, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2022:NGQ

[LYX+22] Zi Li, Yong Yang, Tianlv Xu, Herbert Früchtl, Tanja van Mourik, Martin J. Paterson, Yasuteru Shigeta, Steven R. Kirk, and Samantha Jenkins. Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation.

Journal of Computational Chemistry, 43(3):206–214, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Li:2023:FIS

[LZW+23] Hongmin Li, Yangyu Zhou, Guanjun Wang, Xiaoqing Zeng, and Mingfei Zhou. Formation and infrared spectroscopic characterization of carbon suboxide complexes TM-η^1-C_3O_2 and the inserted ketenylidene complexes OCTMCCO (TM = Cu, Ag, Au) in solid neon. *Journal of Computational Chemistry*, 44(3):129–137, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitsuta:2023:CWN

[MA23a] Yuki Mitsuta and Toshio Asada. Curvature-weighted nudged elastic band method using the Riemann curvature. *Journal of Computational Chemistry*, 44(5):662–669, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mitsuta:2023:NES

[MA23b] Yuki Mitsuta and Toshio Asada. Nudged elastic stiffness band method: a method to solve kinks problems of reaction paths. *Journal of Computational Chemistry*, 44(23):1884–1897, September 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez-Araya:2022:ASC

[MAI22] Jorge I. Martínez-Araya and Rafael Islas. Analysis in silico of chemical reactivity employing the local hyper-softness in some classic aromatic compounds, boron aromatic clusters and all-metal aromatic clusters. *Journal of Computational Chemistry*, 43(1):29–42, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Melse:2023:BBF

[MAKZ23] Okke Melse, Iris Antes, Ville R. I. Kaila, and Martin Zacharias. Benchmarking biomolecular force field-based Zn^{2+} for mono- and bimetallic ligand binding sites. *Journal of Computational Chemistry*, 44(8):912–926, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez-Araya:2021:DPR

[MAM21] Jorge I. Martínez-Araya and Christophe Morell. The density polarization reveals directions of electron displacements due to the substituent effect: Analysis performed on a metal-organic Mo-Oxo catalyst. *Journal of Computational Chemistry*, 42 (16):1118–1125, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maltsev:2023:ICI

[MAM+23] Maxim A. Maltsev, Svetlana A. Aksenova, Igor V. Morozov, Yury Minenkov, and Evgenia L. Osina. Ab initio calculations of the interaction potentials and thermodynamic functions for ArN and ArN^+. *Journal of Computational Chemistry*, 44(12): 1189–1198, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muthusivarajan:2020:RAR

[MAP+20] Rajarajeswari Muthusivarajan, William J. Allen, Ashok D. Pehere, Konstantin V. Sokolov, and David Fuentes. Role of alkylated residues in the tetrapeptide self-assembly — a molecular dynamics study. *Journal of Computational Chemistry*, 41 (31):2634–2640, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marti:2021:QQA

[Mar21] Sergio Martí. QMCube (QM^3): an all-purpose suite for multiscale QM/MM calculations. *Journal of Computational Chemistry*, 42(6):447–457, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mrovec:2021:DFO

[MB21] Martin Mrovec and J. A. Berger. A diagonalization-free optimization algorithm for solving Kohn–Sham equations of closed-shell molecules. *Journal of Computational Chemistry*, 42(7):492–504, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morera-Boado:2023:IEC

[MBBU23] Cercis Morera-Boado and Margarita I. Bernal-Uruchurtu. Interaction energy of Cl_2 and Br_2 with H_2O: Exchange, dispersion and density the crucial ingredients. *Journal of Computa-*

tional Chemistry, 44(10):1073–1087, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

McCutcheon:2023:AMC

[MC23] Jessica N. McCutcheon and D. Allen Clabo, Jr. An atoms-in-molecules characterization of the nature of the O–O bond in peroxides and nitroxide dimers. *Journal of Computational Chemistry*, 44(13):1278–1290, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mondal:2024:CRU

[MC24] Himangshu Mondal and Pratim Kumar Chattaraj. CO_2 reduction using aluminum hydride: Generation of in-situ frustrated Lewis pairs and small molecule activation therein. *Journal of Computational Chemistry*, 45(14):1098–1111, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Munoz-Castro:2022:BCN

[MCD22] Alvaro Muñoz-Castro and H. V. Rasika Dias. Bonding and ^{13}C-NMR properties of coinage metal tris(ethylene) and tris(norbornene) complexes: Evaluation of the role of relativistic effects from DFT calculations. *Journal of Computational Chemistry*, 43(27):1848–1855, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Minenkov:2023:ICB

[MCP23] Yury Minenkov, Luigi Cavallo, and Kirk A. Peterson. Influence of the complete basis set approximation, tight weighted-core, and diffuse functions on the DLPNO-CCSD(T1) atomization energies of neutral H,C,O-compounds. *Journal of Computational Chemistry*, 44(5):687–696, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Madabeni:2020:CMB

[MDO+20] Andrea Madabeni, Marco Dalla Tiezza, Folorunsho Bright Omage, Pablo Andrei Nogara, Marco Bortoli, João Batista Teixeira Rocha, and Laura Orian. Chalcogen-mercury bond formation and disruption in model Rabenstein's reactions: a computational analysis. *Journal of Computational Chemistry*, 41 (23):2045–2054, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Milanez:2023:SSL

[MdSJ+23] Bruno D. Milanez, Gustavo M. dos Santos, Max Pinheiro Jr, Leonardo T. Ueno, Luiz F. A. Ferrão, Adelia J. A. Aquino, Hans Lischka, and Francisco B. C. Machado. Structural stability and the low-lying singlet and triplet states of BN-n-acenes, $n = 1$–7. *Journal of Computational Chemistry*, 44(6):755–765, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matveeva:2022:EMF

[MEKH22] Regina Matveeva, Merete Falck Erichsen, Henrik Koch, and Ida-Marie Høyvik. The effect of midbond functions on interaction energies computed using MP2 and CCSD(T). *Journal of Computational Chemistry*, 43(2):121–131, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malloum:2020:LSA

[MFC20] Alhadji Malloum, Jean J. Fifen, and Jeanet Conradie. Large-sized ammonia clusters and solvation energies of the proton in ammonia. *Journal of Computational Chemistry*, 41(1):21–30, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Medves:2022:ODF

[MFS22] Marco Medves, Giovanna Fronzoni, and Mauro Stener. Optimization of density fitting auxiliary Slater-type basis functions for time-dependent density functional theory. *Journal of Computational Chemistry*, 43(28):1923–1935, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mrovec:2024:HDP

[MG24] Martin Mrovec and Peter M. W. Gill. How delocalized are the polyacenes? *Journal of Computational Chemistry*, 45(11): 701–709, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marcisz:2022:ESR

[MGB+22] Mateusz Marcisz, Margrethe Gaardløs, Krzysztof K. Bojarski, Till Siebenmorgen, Martin Zacharias, and Sergey A. Samsonov. Explicit solvent repulsive scaling replica exchange molecular dynamics (RS-REMD) in molecular modeling of protein-glycosaminoglycan complexes. *Journal of Computational Chemistry*, 43(24):1633–1640, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Merzoud:2021:UID

[MGCM21] Lynda Merzoud, Frédéric Guégan, Henry Chermette, and Christophe Morell. Understanding the intermolecular Diels–Alder cycloaddition promotion: Activation strain model/ energy decomposition analysis model and conceptual density functional theory viewpoints. *Journal of Computational Chemistry*, 42(19):1364–1372, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Miyamoto:2020:SER

[MH20] Masaya Miyamoto and Masahiko Hada. Surface-enhanced Raman scattering of M_2-pyrazine-M_2 (M = Cu, Ag, Au): Analysis by natural perturbation orbitals and density functional theory functional dependence. *Journal of Computational Chemistry*, 41(17):1628–1637, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Macedo:2022:PEC

[MH22] Gabriel Kossaka Macedo and Roberto Luiz Andrade Haiduke. The performance of exchange-correlation functionals in describing electron density parameters of saddle point structures along chemical reactions. *Journal of Computational Chemistry*, 43(27):1830–1838, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Melin:2023:TPP

[MHA+23] Timothé R. L. Melin, Preston Harell, Betoul Ali, Narasimhan Loganathan, and Angela K. Wilson. Thermochemistry of per- and polyfluoroalkyl substances. *Journal of Computational Chemistry*, 44(4):570–580, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mishima:2023:OKH

[MIK+23] Hirokazu Mishima, Yukihiro Itoh, Takashi Kurohara, Takayoshi Suzuki, Naoya Asada, Ken ichi Kusakabe, and Yuko Okamoto. Origin of the kinetic HDAC2-selectivity of an HDAC inhibitor. *Journal of Computational Chemistry*, 44(18):1604–1609, July

5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Milovanovic:2021:SLC

[Mil21] Milan Milovanović. Small lithium-chloride clusters: Superalkalis, superhalogens, supersalts and nanocrystals. *Journal of Computational Chemistry*, 42(26):1895–1904, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Minh:2020:AGD

[Min20] David D. L. Minh. Alchemical Grid Dock (AlGDock): Binding free energy calculations between flexible ligands and rigid receptors. *Journal of Computational Chemistry*, 41(7):715–730, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muya:2021:SSB

[MIP+21] Jules Tshishimbi Muya, Bienfait Kabuyaya Isamura, Issofa Patouossa, Minh Tho Nguyen, and Arnout Ceulemans. Structure, stability and bonding of the leapfrog $B_{24}^{0,\pm1,\pm2}$. *Journal of Computational Chemistry*, 42(2):72–80, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maraf:2022:DRM

[MIP+22] Mbah Bake Maraf, Adjieufack Abel Idrice, Manwal A. Mekoung Pélagie, Auguste Abouem A. Zintchem, Gouet Bebga, Lydia Rhyman, Mbouombouo Ndassa Ibrahim, and Ponnadurai Ramasami. Decoding the reaction mechanism of the cyclocondensation of ethyl acetate2-oxo-2-(4-oxo-4 *H*-pyrido [1.2-a] pyrimidin-3-yl) polyazaheterocycle and ethylenediamine using bond evolution theory. *Journal of Computational Chemistry*, 43(14):972–985, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mondal:2023:SSS

[MJS+23] Sukanta Mondal, Gourhari Jana, Hemant K. Srivastava, Garikapati N. Sastry, and Pratim Kumar Chattaraj. Structure and stability of the sH binary hydrate cavity and host-guest versus guest-guest interactions therein: a DFT approach. *Journal of Computational Chemistry*, 44(15):1446–1453, June

5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Monroe:2022:USM

[MK22a] Lyman Monroe and Daisuke Kihara. Using steered molecular dynamic tension for assessing quality of computational protein structure models. *Journal of Computational Chemistry*, 43 (17):1140–1150, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muz:2022:ZON

[MK22b] Iskender Muz and Mustafa Kurban. Zinc oxide nanoclusters and their potential application as CH_4 and CO_2 gas sensors: Insight from DFT and TD-DFT. *Journal of Computational Chemistry*, 43(27):1839–1847, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Menzel:2021:EWI

[MKB+21] Jan Paul Menzel, Martijn Kloppenburg, Jelena Belić, Huub J. M. de Groot, Lucas Visscher, and Francesco Buda. Efficient workflow for the investigation of the catalytic cycle of water oxidation catalysts: Combining GFN-xTB and density functional theory. *Journal of Computational Chemistry*, 42 (26):1885–1894, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mandal:2022:ISP

[MKK+22] Sagarmoy Mandal, Ritama Kar, Tobias Klöffel, Bernd Meyer, and Nisanth N. Nair. Improving the scaling and performance of multiple time stepping-based molecular dynamics with hybrid density functionals. *Journal of Computational Chemistry*, 43(9):588–597, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsuoka:2020:RTT

[MKSS20] Daisuke Matsuoka, Motoshi Kamiya, Takeshi Sato, and Yuji Sugita. Role of the N-terminal transmembrane helix contacts in the activation of FGFR3. *Journal of Computational Chemistry*, 41(6):561–572, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maley:2023:DFT

[MLB+23] Steven M. Maley, Graham R. Lief, Richard M. Buck, Orson L. Sydora, Qing Yang, Steven M. Bischof, and Daniel H. Ess. Density functional theory and CCSD(T) evaluation of ionization potentials, redox potentials, and bond energies related to zirconocene polymerization catalysts. *Journal of Computational Chemistry*, 44(4):506–515, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2023:MLA

[MLC+23] Yingjin Ma, ZhiYing Li, Xin Chen, Bowen Ding, Ning Li, Teng Lu, Baohua Zhang, BingBing Suo, and Zhong Jin. Machine-learning assisted scheduling optimization and its application in quantum chemical calculations. *Journal of Computational Chemistry*, 44(12):1174–1188, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mao:2021:CI

[MLG+21a] Yuxia Mao, Shiliang Li, Bojie Gong, Luhua Lai, Gaoqi He, and Honglin Li. Cover image. *Journal of Computational Chemistry*, 42(30):i, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mao:2021:EIG

[MLG+21b] Yuxia Mao, Shiliang Li, Bojie Gong, Luhua Lai, Gaoqi He, and Honglin Li. ePharmer: an integrated and graphical software for pharmacophore-based virtual screening. *Journal of Computational Chemistry*, 42(30):2181–2195, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mo:2024:IIB

[MLGY24] Otilia Mó, Al Mokhtar Lamsabhi, Jean-Claude Guillemin, and Manuel Yáñez. Ionization, intrinsic basicity, and intrinsic acidity of unsaturated diols of astrochemical interest: 1,1- and 1,2-ethenediol: a theoretical survey. *Journal of Computational Chemistry*, 45(3):140–149, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manna:2024:IDC

[MLM+24] Debashree Manna, Rabindranath Lo, Vijay Madhav Miriyala, Dana Nachtigallová, Zdenek Trávnícek, and Pavel Hobza. Impact of dielectric constant of solvent on the formation of transition metal-ammine complexes. *Journal of Computational Chemistry*, 45(4):204–209, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Modee:2022:BSD

[MLP22] Rohit Modee, Siddhartha Laghuvarapu, and U. Deva Priyakumar. Benchmark study on deep neural network potentials for small organic molecules. *Journal of Computational Chemistry*, 43(5):308–318, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mi:2024:RMC

[MLX+24] Xiao Peng Mi, Hui Lu, Tianlv Xu, Herbert Früchtl, Tanja van Mourik, Martin J. Paterson, Steven R. Kirk, and Samantha Jenkins. Response of the mechanical and chiral character of ethane to ultra-fast laser pulses. *Journal of Computational Chemistry*, 45(3):150–158, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Marcus:2020:WRS

[MM20] Kendra Marcus and Carla Mattos. Water in Ras superfamily evolution. *Journal of Computational Chemistry*, 41(5):402–414, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mehta:2024:SCP

[MM24] Nisha Mehta and Jan M. L. Martin. On the sensitivity of computed partial charges toward basis set and (exchange-)correlation treatment. *Journal of Computational Chemistry*, 45(13):1017–1032, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Morin-Martinez:2023:QBA

[MMAZ+23] Armando A. Morin-Martinez, Jessica Arcudia, Ximena Zarate, Miguel Eduardo Cifuentes-Quintal, and Gabriel Merino. The quest for a bidirectional auxetic, elastic, and enhanced fracture toughness material: Revisiting the mechanical properties of the BeH_2 monolayers. *Journal of Computational Chemistry*, 44(3):248–255, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maya:2024:QCE

[MMF+24] Josué Maya, Alhadji Malloum, Jean Jules Fifen, Zoubeida Dhaouadi, Henri Paul Ekobena Fouda, and Jeanet Conradie. Quantum cluster equilibrium theory applied to liquid ammonia. *Journal of Computational Chemistry*, 45(15):1279–1288, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mashkovtsev:2020:EMI

[MMK+20] Denis Mashkovtsev, Wataru Mizukami, Jacek Korchowiec, Anna Stachowicz-Ku'snierz, and Yuriko Aoki. Elongation method with intermediate mechanical and electrostatic embedding for geometry optimizations of polymers. *Journal of Computational Chemistry*, 41(25):2203–2212, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2023:RSC

[MML+23] Delong Ma, Song Ma, Yunfeng Li, Jianyong Yuan, Jionghao He, and Shuangliang Zhao. Reactivities of silane coupling agents in the silica/rubber composites: Theoretical insights into the relationships between energy barriers and electronic characteristics. *Journal of Computational Chemistry*, 44(4):581–593, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mandal:2020:ECF

[MN20] Sagarmoy Mandal and Nisanth N. Nair. Efficient computation of free energy surfaces of chemical reactions using ab initio molecular dynamics with hybrid functionals and plane waves. *Journal of Computational Chemistry*, 41(19):1790–1797, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martinez-Nunez:2021:AOS

[MNBG+21] Emilio Martínez-Núñez, George L. Barnes, David R. Glowacki, Sabine Kopec, Daniel Peláez, Aurelio Rodríguez, Roberto Rodríguez-Fernández, Robin J. Shannon, James J. P. Stewart, Pablo G. Tahoces, and Saulo A. Vazquez. AutoMeKin2021: an open-source program for automated reaction discovery. *Journal of Computational Chemistry*, 42(28):2036–2048, October

30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2021:IES

[MNH21] Zhifeng Ma, Naoki Nakatani, and Masahiko Hada. Insights into the electronic structure and mechanism of norcarane hydroxylation by OxoMn(V) porphyrin complexes: a density functional theory study. *Journal of Computational Chemistry*, 42(27):1920–1928, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mancera:2020:DAR

[MNZGO+20] Jennifer Paola Hernández Mancera, Francisco Núñez-Zarur, Soledad Gutiérrez-Oliva, Alejandro Toro-Labbé, and Ricardo Vivas-Reyes. Diels–Alder reaction mechanisms of substituted chiral anthracene: a theoretical study based on the reaction force and reaction electronic flux. *Journal of Computational Chemistry*, 41(23):2022–2032, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mondal:2024:DGS

[Mon24] Sukanta Mondal. β-D-glucopyranose-silver+ (1:1) complex as a small gas molecule scavenger. *Journal of Computational Chemistry*, 45(17):1434–1443, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muhasina:2023:VRT

[MP23] Puthan Veetil Muhasina and Pattiyil Parameswaran. σ versus π-radical: Tuning the electronic nature of neutral carbon (I) compounds with three non-bonding electrons. *Journal of Computational Chemistry*, 44(3):422–431, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Manchev:2024:FMS

[MP24] Yulian T. Manchev and Paul L. A. Popelier. `FFLUX` molecular simulations driven by atomic Gaussian process regression models. *Journal of Computational Chemistry*, 45(15):1235–1246, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mendanha:2021:MDS

[MPOC21] Karinna Mendanha, Richard Costa Prado, Leonardo Bruno Assis Oliveira, and Guilherme Colherinhas. Molecular dynamic simulations, GIAO-NMR and TD-DFT spectroscopy analyze for zwitterionic isoleucine $(\mathrm{ILE})_N$, $1 \leq N \leq 6$, in water solution. *Journal of Computational Chemistry*, 42(5):344–357, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Macchiagodena:2023:RPT

[MPP23] Marina Macchiagodena, Marco Pagliai, and Piero Procacci. NE-RDFE: a protocol and toolkit for computing relative dissociation free energies with GROMACS between dissimilar molecules using bidirectional nonequilibrium dual topology schemes. *Journal of Computational Chemistry*, 44(12):1221–1230, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mathea:2022:AVC

[MPR22] Tina Mathea, Taras Petrenko, and Guntram Rauhut. Advances in vibrational configuration interaction theory — part 2: Fast screening of the correlation space. *Journal of Computational Chemistry*, 43(1):6–18, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malik:2020:HWS

[MPuS+20] Aijaz Ahmad Malik, Chuleeporn Phanus-umporn, Nalini Schaduangrat, Watshara Shoombuatong, Chartchalerm Isarankura-Na-Ayudhya, and Chanin Nantasenamat. HCVpred: a web server for predicting the bioactivity of hepatitis C virus NS5B inhibitors. *Journal of Computational Chemistry*, 41(20):1820–1834, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mifkovic:2022:CPP

[MPV22] Maleigh Mifkovic, Jessica Pauling, and Shubham Vyas. Computational protocol for predicting ^{19}F NMR chemical shifts for PFAS and connection to PFAS structure. *Journal of Computational Chemistry*, 43(20):1355–1361, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mathea:2021:AVC

[MR21] Tina Mathea and Guntram Rauhut. Advances in vibrational configuration interaction theory — part 1: Efficient calculation of vibrational angular momentum terms. *Journal of Computational Chemistry*, 42(32):2321–2333, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mollahosseini:2022:EMI

[MSA22a] Arash Mollahosseini, Shaghayegh Saadati, and Amira Abdelrasoul. Effects of mussel-inspired co-deposition of 2-hydroxymethyl methacrylate and poly (2-methoxyethyl acrylate) on the hydrophilicity and binding tendency of common hemodialysis membranes: Molecular dynamics simulations and molecular docking studies. *Journal of Computational Chemistry*, 43(1):57–73, January 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Monti:2022:CAM

[MSA22b] Marta Monti, Mauro Stener, and Massimiliano Aschi. A computational approach for modeling electronic circular dichroism of solvated chromophores. *Journal of Computational Chemistry*, 43(30):2023–2036, November 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matsuoka:2024:EED

[MSA$^+$24] Sota Matsuoka, Kota Sakakura, Yoshinobu Akinaga, Kazuki Akisawa, Koji Okuwaki, Hideo Doi, and Yuji Mochizuki. Enhancement of energy decomposition analysis in fragment molecular orbital calculations. *Journal of Computational Chemistry*, 45(12):898–902, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mkadmh:2021:SID

[MSE$^+$21] Ahmed M. Mkadmh, Zaki S. Safi, Adnan A. Elkhaldy, Richard J. Staples, Savas Kaya, and Goncagül Serdaroglu. Synthesis, identification, density functional and Hirshfeld surface studies of 2,2'-disulfanediylbis(tetrahydro-4*H*-cyclopenta[*d*][1,3,2]dioxaphosphole-2-sulfide). *Journal of Computational Chemistry*, 42(26):1873–1884, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Martino:2020:CPE

[MSL+20] Marta Martino, Andrea Salvadori, Federico Lazzari, Lorenzo Paoloni, Surajit Nandi, Giordano Mancini, Vincenzo Barone, and Sergio Rampino. Chemical promenades: Exploring potential-energy surfaces with immersive virtual reality. *Journal of Computational Chemistry*, 41(13):1310–1323, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Muller:2020:RTT

[MSS20] Carolin Müller, Manas Sharma, and Marek Sierka. Real-time time-dependent density functional theory using density fitting and the continuous fast multipole method. *Journal of Computational Chemistry*, 41(30):2573–2582, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mazumder:2023:BBN

[MSYS23] Lakhya Jyoti Mazumder, Rohan Sharma, Farnaz Yashmin, and Pankaz Kumar Sharma. Beryllium bonding with noble gas atoms. *Journal of Computational Chemistry*, 44(4):644–655, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahajan:2019:MCG

[MT19] 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 [MT20a].

Mahajan:2020:EMC

[MT20a] 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 [MT19].

Mukhopadhyay:2020:ENR

[MT20b] Roma Mukhopadhyay and Marat R. Talipov. Efficient Newton–Raphson/singular value decomposition-based optimization scheme with dynamically updated critical condition number for rapid convergence of weighted histogram analysis method equations. *Journal of Computational Chemistry*, 41(3):240–246, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mahajan:2021:CMF

[MT21] Subhamoy Mahajan and Tian Tang. Comment on "Martini force field for protonated polyethyleneimine". *Journal of Computational Chemistry*, 42(4):261–263, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Malcek:2020:CBD

[MVP+20] Michal Malcek, Barbora Vénosová, Ingrid Puskárová, Jozef Kozísek, Marián Gall, and Lukás Bucinský. Coordination bonding in dicopper and dichromium tetrakis(μ-acetato)-diaqua complexes: Nature, strength, length, and topology. *Journal of Computational Chemistry*, 41(7):698–714, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Mifkovic:2022:CDH

[MVV22] Maleigh Mifkovic, Daniel J. Van Hoomissen, and Shubham Vyas. Conformational distributions of helical perfluoroalkyl substances and impacts on stability. *Journal of Computational Chemistry*, 43(24):1656–1661, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ma:2020:PPP

[MWK+20] He Ma, Wennie Wang, Siyoung Kim, Man-Hin Cheng, Marco Govoni, and Giulia Galli. PyCDFT: a Python package for constrained density functional theory. *Journal of Computational Chemistry*, 41(20):1859–1867, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Menzer:2020:REP

[MXM20] William M. Menzer, Bing Xie, and David D. L. Minh. On restraints in end-point protein-ligand binding free energy calculations. *Journal of Computational Chemistry*, 41(6):573–586, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maruyama:2024:RSP

[MY24] Yutaka Maruyama and Norio Yoshida. `RISMiCal`: a software package to perform fast RISM/3D-RISM calculations. *Journal of Computational Chemistry*, 45(17):1470–1482, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Meraz:2024:PCA

[MYYS24] Md Mostakim Meraz, Wenhong Yang, Weisheng Yang, and Wen-Hua Sun. Predicting the catalytic activities of transition metal (Cr, Fe, Co, Ni) complexes towards ethylene polymerization by machine learning. *Journal of Computational Chemistry*, 45(11):798–803, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Matyszczak:2021:AAN

[MZ21] Grzegorz Matyszczak and Krzysztof Zberecki. Application of artificial neural network and global optimization techniques for high throughput modeling of the crystal structure of stannites and kesterites. *Journal of Computational Chemistry*, 42 (11):740–745, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Maszota-Zieleniak:2021:ERE

[MZMK+21] Martyna Maszota-Zieleniak, Mateusz Marcisz, Małgorzata M. Kogut, Till Siebenmorgen, Martin Zacharias, and Sergey A. Samsonov. Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. *Journal of Computational Chemistry*, 42(15):1040–1053, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nair:2021:RAO

[NAAP21] Akhil S. Nair, Anakuthil Anoop, Rajeev Ahuja, and Biswarup Pathak. Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: a global optimization study. *Journal of Computational Chemistry*, 42(27): 1944–1958, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakamura:2023:STA

[NAN+23] Shinya Nakamura, Tatsuo Akaki, Keiji Nishiwaki, Midori Nakatani, Yuji Kawase, Yuki Takahashi, and Isao Nakanishi. System truncation accelerates binding affinity calculations with the fragment molecular orbital method: a benchmark study. *Journal of Computational Chemistry*, 44(7):824–831, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nanni:2024:IPT

[Nan24] Luca Nanni. Investigating proton tunneling dynamics in the time-dependent Schrödinger equation. *Journal of Computational Chemistry*, 45(18):1614–1623, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neugebauer:2023:HTS

[NBE+23] Hagen Neugebauer, Benedikt Bädorf, Sebastian Ehlert, Andreas Hansen, and Stefan Grimme. High-throughput screening of spin states for transition metal complexes with spin-polarized extended tight-binding methods. *Journal of Computational Chemistry*, 44(27):2120–2129, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Novotny:2024:TAM

[NDK24] Michal Novotný, Matús Dubecký, and Frantisek Karlický. Toward accurate modeling of structure and energetics of bulk hexagonal boron nitride. *Journal of Computational Chemistry*, 45(2):115–121, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Neese:2023:SIG

[Nee23] Frank Neese. The SHARK integral generation and digestion system. *Journal of Computational Chemistry*, 44(3):381–396, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nelson:2020:LLO

[NEG+20] Ryky Nelson, Christina Ertural, Janine George, Volker L. Deringer, Geoffroy Hautier, and Richard Dronskowski. LOBSTER: Local orbital projections, atomic charges, and chemical-bonding analysis from projector-augmented-wave-based density-functional theory. *Journal of Computational Chemistry*, 41(21):1931–1940, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Najibi:2020:DDC

[NG20] Asim Najibi and Lars Goerigk. DFT-D4 counterparts of leading meta-generalized-gradient approximation and hybrid density functionals for energetics and geometries. *Journal of Computational Chemistry*, 41(30):2562–2572, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nikolaienko:2022:CML

[NGD22] Tymofii Nikolaienko, Oleksandr Gurbych, and Maksym Druchok. Complex machine learning model needs complex testing: Examining predictability of molecular binding affinity by a graph neural network. *Journal of Computational Chemistry*, 43(10):728–739, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ngo:2021:ELB

[Ngo21] Son Tung Ngo. Estimating the ligand-binding affinity via λ-dependent umbrella sampling simulations. *Journal of Computational Chemistry*, 42(2):117–123, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakatani:2021:AVE

[NHFS21] Kaho Nakatani, Masahiro Higashi, Ryoichi Fukuda, and Hirofumi Sato. An analysis of valence electronic structure from a viewpoint of resonance theory: Tautomerization of formamide and diazadiboretidine. *Journal of Computational Chemistry*, 42(23):1662–1669, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2022:BCC

[NI22] Anh L. P. Nguyen and Ekaterina I. Izgorodina. Behavior of counterpoise correction in many-body molecular clusters of organic compounds: Hartree–Fock interaction energy perspective. *Journal of Computational Chemistry*, 43(8):568–576, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nam:2023:SSP

[NLC23] Youhyun Nam, Songyi Lee, and Rakwoo Chang. Structure and stability of polydiacetylene membrane systems: Molecular dynamics simulation studies. *Journal of Computational Chemistry*, 44(8):927–934, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2021:PLE

[NMFI21] Anh L. P. Nguyen, Thomas G. Mason, Benny D. Freeman, and Ekaterina I. Izgorodina. Prediction of lattice energy of benzene crystals: a robust theoretical approach. *Journal of Computational Chemistry*, 42(4):248–260, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nikitin:2021:FCS

[NML21] Alexei Nikitin, Vladislava Milchevskaya, and Alexander Lyubartsev. To the fast calculation of the solvation free energy. Combining expanded ensembles with L2MC. *Journal of Computational Chemistry*, 42(11):787–792, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nacereddine:2021:CIS

[NMMC21] Abdelmalek Khorief Nacereddine, Lynda Merzoud, Christophe Morell, and Henry Chermette. A computational investigation of the selectivity and mechanism of the Lewis acid catalyzed oxa-Diels–Alder cycloaddition of substituted diene with benzaldehyde. *Journal of Computational Chemistry*, 42(18): 1296–1311, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nishimura:2020:HPD

[NN20] Yoshifumi Nishimura and Hiromi Nakai. Hierarchical parallelization of divide-and-conquer density functional tight-binding molecular dynamics and metadynamics simulations. *Journal of Computational Chemistry*, 41(19):1759–1772, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ngo:2020:OFE

[NNT+20] Son Tung Ngo, Trung Hai Nguyen, Nguyen Thanh Tung, Pham Cam Nam, Khanh B. Vu, and Van V. Vu. Oversampling free energy perturbation simulation in determination of the ligand-binding free energy. *Journal of Computational Chemistry*, 41(7):611–618, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nourian:2023:IPR

[NP23] Pouria Nourian and Andrew J. Peters. Implementation of probe rheology simulation technique in atomistically detailed molecular dynamics simulations. *Journal of Computational Chemistry*, 44(16):1484–1492, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Novak:2023:DCD

[NPGP23] Jurica Novak, Prateek Pathak, Maria A. Grishina, and Vladimir A. Potemkin. The design of compounds with desirable properties — the anti-HIV case study. *Journal of Computational Chemistry*, 44(10):1016–1030, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Narsaria:2020:PTV

[NRH+20] Ayush K. Narsaria, Julian D. Ruijter, Trevor A. Hamlin, Andreas W. Ehlers, Célia Fonseca Guerra, Koop Lammertsma, and F. Matthias Bickelhaupt. Performance of TDDFT vertical excitation energies of core-substituted naphthalene diimides. *Journal of Computational Chemistry*, 41(15):1448–1455, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nag:2022:SHM

[NS22] Shubhadeep Nag and Yashonath Subramanian. Separation of hydrocarbon mixture of neopentane and n-hexane using NaY zeolite: Large distinct diffusivity. *Journal of Computational Chemistry*, 43(10):660–673, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nash:2023:CCA

[NSH23] Harry W. Nash, Robert A. Shaw, and John Grant Hill. Correlation consistent auxiliary basis sets in density fitting Hartree–

Fock: The atoms sodium through argon revisited. *Journal of Computational Chemistry*, 44(11):1119–1128, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nhat:2021:ALE

[NSKN21] Pham Vu Nhat, Nguyen Thanh Si, Vitaly G. Kiselev, and Minh Tho Nguyen. Another look at energetically quasi-degenerate structures of the gold cluster Au_{27}^{q} with $q = 1, 0, -1$. *Journal of Computational Chemistry*, 42(30):2145–2153, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakov:2021:PAA

[NSRK21] Svetoslav Nakov, Ekaterina Sobakinskaya, Thomas Renger, and Johannes Kraus. `ARGOS`: an adaptive refinement goal-oriented solver for the linearized Poisson–Boltzmann equation. *Journal of Computational Chemistry*, 42(26):1832–1860, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nhat:2020:EBM

[NST+20] Pham Vu Nhat, Nguyen Thanh Si, Nguyen Thi Thu Tram, Long Van Duong, and Minh Tho Nguyen. Elucidating the binding mechanism of thione-containing mercaptopurine and thioguanine drugs to small gold clusters. *Journal of Computational Chemistry*, 41(19):1748–1758, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nanayakkara:2021:CEN

[NTK21] Sadisha Nanayakkara, Yunwen Tao, and Elfi Kraka. Comment on "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*, 42(7):516–521, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nakamura:2021:CGE

[NUK21] Taiji Nakamura, Tamotsu Uchiyama, and Takako Kudo. Comparison of group 14 elements in sp^3 and sp^2 environment by fragment structure energy analysis. *Journal of Computational*

Chemistry, 42(25):1817–1825, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nieuwland:2023:UCS

[NVBG23] Celine Nieuwland, Pascal Vermeeren, F. Matthias Bickelhaupt, and Célia Fonseca Guerra. Understanding chemistry with the symmetry-decomposed Voronoi deformation density charge analysis. *Journal of Computational Chemistry*, 44(27): 2108–2119, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Nguyen:2022:TMT

[NYM22] Catrina Nguyen, Lauren M. Yearwood, and Michelle E. McCully. Thermostabilization mechanisms in thermophilic versus mesophilic three-helix bundle proteins. *Journal of Computational Chemistry*, 43(3):197–205, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

ODonnell:2023:GCW

[OAC23] Timothée O'Donnell, Viraj Agashe, and Frédéric Cazals. Geometric constraints within tripeptides and the existence of tripeptide reconstructions. *Journal of Computational Chemistry*, 44(13):1236–1249, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ozuguzel:2023:RRS

[OAN+23] Umut Ozuguzel, Adelia J. A. Aquino, Reed Nieman, Shelley D. Minteer, and Carol Korzeniewski. Resonance Raman spectra and excited state properties of methyl viologen and its radical cation from time-dependent density functional theory. *Journal of Computational Chemistry*, 44(31):2414–2423, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

ODonnell:2023:ECE

[OC23] Timothée O'Donnell and Frédéric Cazals. Enhanced conformational exploration of protein loops using a global parameterization of the backbone geometry. *Journal of Computational Chemistry*, 44(11):1094–1104, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orabi:2020:DPF

[ODL20] Esam A. Orabi, Rebecca L. Davis, and Guillaume Lamoureux. Drude polarizable force field for cation–π interactions of alkali and quaternary ammonium ions with aromatic amino acid side chains. *Journal of Computational Chemistry*, 41(5):472–481, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orangi:2020:FLA

[OE20] Nasim Orangi and Kiamars Eskandari. Fluorine as a Lewis acid: a symmetry-adapted perturbation theory based on density functional theory and interacting quantum atoms study of noncovalent interactions in the NCF$\cdots$$NH_3$ complex. *Journal of Computational Chemistry*, 41(17):1598–1605, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohno:2021:HPG

[OKI+21] Koichi Ohno, Naoki Kishimoto, Takeaki Iwamoto, Hiroko Satoh, and Hiromasa Watanabe. High performance global exploration of isomers and isomerization channels on quantum chemical potential energy surface of $H_5C_2NO_2$. *Journal of Computational Chemistry*, 42(3):192–204, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Omodemi:2022:PIP

[OKK22] Oluwaseun Omodemi, Martina Kaledin, and Alexey L. Kaledin. Permutationally invariant polynomial representation of polarizability tensor surfaces for linear regression analysis. *Journal of Computational Chemistry*, 43(22):1495–1503, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohlknecht:2020:CEA

[ÖLP+20] Christoph Öhlknecht, Bettina Lier, Drazen Petrov, Julian Fuchs, and Chris Oostenbrink. Correcting electrostatic artifacts due to net-charge changes in the calculation of ligand binding free energies. *Journal of Computational Chemistry*, 41(10):986–999, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otlyotov:2022:CEM

[OM22] Arseniy A. Otlyotov and Yury Minenkov. Conformational energies of microsolvated Na^+ clusters with protic and aprotic solvents from GFN *n*-xTB methods. *Journal of Computational Chemistry*, 43(27):1856–1863, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Otlyotov:2023:GPT

[OM23] Arseniy A. Otlyotov and Yury Minenkov. Gas-phase thermochemistry of noncovalent ligand-alkali metal ion clusters: an impact of low frequencies. *Journal of Computational Chemistry*, 44(22):1807–1816, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ottochian:2020:DHT

[OMC+20] Alistar Ottochian, Carmela Morgillo, Ilaria Ciofini, Michael J. Frisch, Giovanni Scalmani, and Carlo Adamo. Double hybrids and time-dependent density functional theory: an implementation and benchmark on charge transfer excited states. *Journal of Computational Chemistry*, 41(13):1242–1251, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See comment [CPG21].

Omotuyi:2020:ASR

[ONA+20] I. Olaposi Omotuyi, Oyekanmi Nash, O. Basiru Ajiboye, C. Gift Iwegbulam, E. Babatunji Oyinloye, O. Abimbola Oyedeji, Z. Abimbola Kashim, and Kunle Okaiyeto. Atomistic simulation reveals structural mechanisms underlying D614G spike glycoprotein-enhanced fitness in SARS-COV-2. *Journal of Computational Chemistry*, 41(24):2158–2161, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orjan:2020:CDG

[ONC20] Erik M. Orján, András B. Nacsa, and Gábor Czakó. Conformers of dehydrogenated glycine isomers. *Journal of Computational Chemistry*, 41(22):2001–2014, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ohno:2020:QCE

[OOY20] Koichi Ohno, Takuto Oki, and Hideo Yamakado. Quantum chemical exploration of intermolecular reactions of acetylene. *Journal of Computational Chemistry*, 41(7):687–697, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Orekhov:2024:CCD

[Ore24] M. A. Orekhov. Correcting charge distribution in reduced Li-molecule pair for computational screening of battery solvents. *Journal of Computational Chemistry*, 45(4):197–203, February 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ootani:2020:TFM

[OSHT20] Yusuke Ootani, Aya Satoh, Yu Harabuchi, and Tetsuya Taketsugu. Trajectory on-the-fly molecular dynamics approach to tunneling splitting in the electronic excited state: a case of tropolone. *Journal of Computational Chemistry*, 41(16):1549–1556, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ozen:2020:TSA

[OSM20] Cihan Ozen, Toshifumi Satoh, and Satoshi Maeda. A theoretical study on the alkali metal carboxylate-promoted L-lactide polymerization. *Journal of Computational Chemistry*, 41(25): 2197–2202, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Oestereich:2024:DED

[OTZW24] Toni Oestereich, Ralf Tonner-Zech, and Julia Westermayr. Decoding energy decomposition analysis: Machine-learned insights on the impact of the density functional on the bonding analysis. *Journal of Computational Chemistry*, 45(7):368–376, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

PhD:2020:SSS

[PAF+20] Sergey S. Akimenko PhD, Galina D. Anisimova, Anastasiya I. Fadeeva, Vasiliy F. Fefelov PhD, Vitaliy A. Gorbunov PhD, Tatyana R. Kayumova, Alexander V. Myshlyavtsev Prof, Marta D. Myshlyavtseva Prof, and Pavel V. Stishenko

PhD. SuSMoST: Surface science modeling and simulation toolkit. *Journal of Computational Chemistry*, 41(23):2084–2097, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2023:FNS

[Pan23] Cong Pan. A formula and numerical study on Ewald 1D summation. *Journal of Computational Chemistry*, 44(8):902–911, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patel:2020:DCI

[PAS+20] Neha Patel, Minhajul Arfeen, Tejender Singh, Shweta Bhagat, Ajay Sakhare, and Prasad V. Bharatam. Divalent N^I compounds: Identifying new carbocyclic carbenes to design nitreones using quantum chemical methods. *Journal of Computational Chemistry*, 41(31):2624–2633, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petrus:2020:PGA

[PB20] Enric Petrus and Carles Bo. Performance of group additivity methods for predicting the stability of uranyl complexes. *Journal of Computational Chemistry*, 41(11):1124–1129, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Parkman:2021:CNP

[PBM21] Jacob A. Parkman, Caleb A. Barksdale, and David J. Michaelis. CAN: a new program to streamline preparation of molecular coordinate files for molecular dynamics simulations. *Journal of Computational Chemistry*, 42(28):2031–2035, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Palmeiro:2021:EM

[PC21] Raúl Palmeiro and Obis Castaño. [10]annulene: Electrocyclization mechanisms. *Journal of Computational Chemistry*, 42(16):1150–1158, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pal:2023:EIR

[PC23] Ranita Pal and Pratim Kumar Chattaraj. Electrophilicity index revisited. *Journal of Computational Chemistry*, 44(3): 278–297, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patel:2024:PES

[PCB+24] Prajay Patel, Joseph Chung, Max Aksel Bowman, Inga Ulusoy, and Angela K. Wilson. Potential energy surfaces and dynamic properties via ab initio composite and density functional approaches. *Journal of Computational Chemistry*, 45 (16):1352–1363, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Porwal:2023:HEV

[PCI23] Vishal Kumar Porwal, Antoine Carof, and Francesca Ingrosso. Hydration effects on the vibrational properties of carboxylates: From continuum models to QM/MM simulations. *Journal of Computational Chemistry*, 44(23):1898–1911, September 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Panthi:2023:AAS

[PDC23] Bhavana Panthi, Saheb Dutta, and Amalendu Chandra. All-atom simulations of the trimeric spike protein of SARS-CoV-2 in aqueous medium: Nature of interactions, conformational stability and free energy diagrams for conformational transition of the protein. *Journal of Computational Chemistry*, 44(17):1560–1577, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pascale:2022:SOS

[PDGD22] Fabien Pascale, Philippe D'Arco, Francesco Silvio Gentile, and Roberto Dovesi. Strategies for the optimization of the structure of crystalline compounds. *Journal of Computational Chemistry*, 43(3):184–196, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pascale:2023:HDC

[PDGD23] Fabien Pascale, Klaus Doll, Francesco Silvio Gentile, and Roberto Dovesi. How deeply are core electrons perturbed when valence electrons are spin polarized? The case study of transition metal compounds. *Journal of Computational Chemistry*, 44(2):65–75, January 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pechlaner:2021:MAB

[PDL+21] Maria Pechlaner, Andreas P. Dorta, Zhixiong Lin, Victor H. Rusu, and Wilfred F. van Gunsteren. A method to apply bond-angle constraints in molecular dynamics simulations. *Journal of Computational Chemistry*, 42(6):418–434, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pascale:2024:JTD

[PDLD24] F. Pascale, P. D'Arco, S. Lebègue, and R. Dovesi. Jahn–Teller distortion, octahedra rotations and orbital ordering in perovskites: KScF as a model system. *Journal of Computational Chemistry*, 45(14):1067–1077, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Petrova:2024:IML

[PDP+24] Vlada V. Petrova, Anton V. Domnin, Yuri B. Porozov, Pavel O. Kuliaev, and Yaroslav V. Solovev. Implementation of machine learning protocols to predict the hydrolysis reaction properties of organophosphorus substrates using descriptors of electron density topology. *Journal of Computational Chemistry*, 45(3):170–182, January 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pagola:2021:PAG

[PFP+21] Gabriel I. Pagola, Marta B. Ferraro, Patricio F. Provasi, Stefano Pelloni, and Paolo Lazzeretti. Physical achirality in geometrically chiral rotamers of hydrazine and boranylborane molecules. *Journal of Computational Chemistry*, 42(25):1772–1782, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pinto:2021:MCP

[PFPD21] Éderson Sales Moreira Pinto, Bruno César Feltes, Conrado Pedebos, and Márcio Dorn. Modifying the catalytic preference of alpha-amylase toward *n*-alkanes for bioremediation purposes using *in silico* strategies. *Journal of Computational Chemistry*, 42(22):1540–1551, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Per:2020:RRS

[PFSC20] Manolo C. Per, Emily K. Fletcher, Ellen T. Swann, and Deidre M. Cleland. Reliable radical stabilization energies from diffusion Monte Carlo calculations. *Journal of Computational Chemistry*, 41(27):2378–2382, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pascale:2024:BGJ

[PGDD24] F. Pascale, S. Gueddida, K. Doll, and R. Dovesi. Band gap, Jahn–Teller deformation, octahedra rotation in transition metal perovskites LaTiO. *Journal of Computational Chemistry*, 45(10):683–694, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Plett:2024:CEB

[PGH24] Christoph Plett, Stefan Grimme, and Andreas Hansen. Conformational energies of biomolecules in solution: Extending the MPCONF196 benchmark with explicit water molecules. *Journal of Computational Chemistry*, 45(7):419–429, March 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Platonenko:2021:ICD

[PGP+21] Alexander Platonenko, Francesco Silvio Gentile, Fabien Pascale, Philippe D'Arco, and Roberto Dovesi. Interstitial carbon defects in silicon. A quantum mechanical characterization through the infrared and Raman spectra. *Journal of Computational Chemistry*, 42(12):806–817, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Perumalla:2023:RDM

[PGP+23] D. Sravanakumar Perumalla, Sagar Ghorai, Tanmoy Pal, Drahomír Hnyk, Josef Holub, and Eluvathingal D. Jemmis. Rearrangement of dicarboranyl methyl cation to icosahedral $C_3B_9H_{12}^+$: an ab initio dynamics view. *Journal of Computational Chemistry*, 44(3):256–260, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pech:2020:QCT

[PHS+20] Cecilia Gomez Pech, Pi A. B. Haase, Dumitru-Claudiu Sergentu, Anastasia Borschevsky, Julien Pilmé, Nicolas Galland,

and Rémi Maurice. Quantum chemical topology at the spin-orbit configuration interaction level: Application to astatine compounds. *Journal of Computational Chemistry*, 41(23): 2055–2065, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pilme:2020:QCT

[Pil20] Julien Pilmé. Quantum chemical topology from tight augmented core densities. *Journal of Computational Chemistry*, 41(17):1616–1627, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Park:2023:ACS

[PJJL23] Jimin Park, InSuk Joung, Keehyoung Joo, and Jooyoung Lee. Application of conformational space annealing to the protein structure modeling using cryo-EM maps. *Journal of Computational Chemistry*, 44(30):2332–2346, November 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Popov:2021:LPP

[PKT21] Ilya V. Popov, Timofei S. Kushnir, and Andrei L. Tchougréeff. Local perturbations of periodic systems. Chemisorption and point defects by `GoGreenGo`. *Journal of Computational Chemistry*, 42(32):2352–2368, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Poleto:2022:TEF

[PL22] Marcelo D. Polêto and Justin A. Lemkul. TUPÃ: Electric field analyses for molecular simulations. *Journal of Computational Chemistry*, 43(16):1113–1119, June 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2020:TSF

[PLP+20] Cong Pan, Chengwen Liu, Junhui Peng, Pengyu Ren, and Xuhui Huang. Three-site and five-site fixed-charge water models compatible with AMOEBA force field. *Journal of Computational Chemistry*, 41(10):1034–1044, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pomogaeva:2024:SSI

[PLT24] Anna V. Pomogaeva, Anna S. Lisovenko, and Alexey Y. Timoshkin. Structures and stability of I_2 and ICl complexes with pyridine: Ab initio and DFT study. *Journal of Computational Chemistry*, 45(12):903–914, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pomogaeva:2023:LAS

[PLZT23] Anna V. Pomogaeva, Anna S. Lisovenko, Artem S. Zavgorodnii, and Alexey Y. Timoshkin. Lewis acid stabilized group 13–15 element analogs of ethylene. *Journal of Computational Chemistry*, 44(3):218–228, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Priyadarsini:2021:CFP

[PM21] Adyasa Priyadarsini and Bhabani S. Mallik. Comparative first principles-based molecular dynamics study of catalytic mechanism and reaction energetics of water oxidation reaction on 2D-surface. *Journal of Computational Chemistry*, 42 (16):1138–1149, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Perron:2022:DGM

[PMT+22] Quentin Perron, Olivier Mirguet, Hamza Tajmouati, Adam Skiredj, Anne Rojas, Arnaud Gohier, Pierre Ducrot, Marie-Pierre Bourguignon, Patricia Sansilvestri-Morel, Nicolas Do Huu, Françoise Gellibert, and Yann Gaston-Mathé. Deep generative models for ligand-based de novo design applied to multi-parametric optimization. *Journal of Computational Chemistry*, 43(10):692–703, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pham:2022:ILR

[PNT+22] T. Ngoc Han Pham, Trung Hai Nguyen, Nguyen Minh Tam, Thien Y. Vu, Nhat Truong Pham, Nguyen Truong Huy, Binh Khanh Mai, Nguyen Thanh Tung, Minh Quan Pham, Van V. Vu, and Son Tung Ngo. Improving ligand-ranking of `AutoDock Vina` by changing the empirical parameters. *Journal of Computational Chemistry*, 43(3):160–169, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Piotrowski:2022:AVW

[POPGS22] Maurício J. Piotrowski, Renato P. Orenha, Renato L. T. Parreira, and Diego Guedes-Sobrinho. Assessment of the van der Waals, Hubbard U parameter and spin-orbit coupling corrections on the 2D/3D structures from metal gold congeners clusters. *Journal of Computational Chemistry*, 43(4):230–243, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pechlaner:2021:UMT

[POvG21] Maria Pechlaner, Chris Oostenbrink, and Wilfred F. van Gunsteren. On the use of multiple-time-step algorithms to save computing effort in molecular dynamics simulations of proteins. *Journal of Computational Chemistry*, 42(18):1263–1282, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pooja:2023:OSS

[PP23] Pooja and Ravinder Pawar. Origin of structure and stability of M@C_{18} (M = Cu, Ag, and Au) complexes with D_{9h} point group. *Journal of Computational Chemistry*, 44(21): 1786–1794, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pagola:2023:ACL

[PPFL23] G. I. Pagola, P. F. Provasi, M. B. Ferraro, and P. Lazzeretti. On the axial chirality of leucoindigo. *Journal of Computational Chemistry*, 44(17):1578–1586, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

PhD:2021:INI

[PPP21] Surjeet Verma PhD, Chirag N. Patel PhD, and Muktesh Chandra PhD. Identification of novel inhibitors of SARS-CoV-2 main protease (m^{pro}) from *Withania* sp. by molecular docking and molecular dynamics simulation. *Journal of Computational Chemistry*, 42(26):1861–1872, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pramanik:2022:MIK

[PPRS22] Debabrata Pramanik, Aiswarya B. Pawar, Sudip Roy, and Jayant Kumar Singh. Mechanistic insights of key host proteins and potential repurposed inhibitors regulating SARS-

CoV-2 pathway. *Journal of Computational Chemistry*, 43(18): 1237–1250, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ponte:2020:MPR

[PPSP20] Fortuna Ponte, GiovanniMaria Piccini, Emilia Sicilia, and Michele Parrinello. A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. *Journal of Computational Chemistry*, 41(4):290–294, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pal:2021:MFB

[PPV+21] Asit Pal, Subhendu Pal, Shivani Verma, Motoyuki Shiga, and Nisanth N. Nair. Mean force based temperature accelerated sliced sampling: Efficient reconstruction of high dimensional free energy landscapes. *Journal of Computational Chemistry*, 42(28):1996–2003, October 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Paiva:2020:AVD

[PRF20] Pedro Paiva, Maria J. Ramos, and Pedro A. Fernandes. Assessing the validity of DLPNO-CCSD(T) in the calculation of activation and reaction energies of ubiquitous enzymatic reactions. *Journal of Computational Chemistry*, 41(29):2459–2468, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pakdel:2020:ESA

[PRH20] Majid Pakdel, Heidar Raissi, and Seyede T. Hosseini. Evaluation the synergistic antitumor effect of methotrexate-camptothecin codelivery prodrug from self-assembly process to acid-catalyzed both drugs release: a comprehensive theoretical study. *Journal of Computational Chemistry*, 41(16): 1486–1496, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Park:2024:SCG

[PRIP24] Soohyung Park, Amy Rice, Wonpil Im, and Richard W. Pastor. Spontaneous curvature generation by peptides in asymmetric bilayers. *Journal of Computational Chemistry*, 45(9): 512–522, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Putro:2023:QMA

[PSA+23] Permono Adi Putro, Aditya Wibawa Sakti, Faozan Ahmad, Hiromi Nakai, and Husin Alatas. Quantum mechanical assessment on the optical properties of capsanthin conformers. *Journal of Computational Chemistry*, 44(30):2319–2331, November 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prentis:2022:MEA

[PSB+22] Lauren E. Prentis, Courtney D. Singleton, John D. Bickel, William J. Allen, and Robert C. Rizzo. A molecular evolution algorithm for ligand design in DOCK. *Journal of Computational Chemistry*, 43(29):1942–1963, November 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prasanna:2021:DOS

[PSGL21] Krishnamohan G. Prasanna, Rahul Sunil, Kapil Gupta, and Seung-Cheol Lee. DJMol: an open-source modeling platform for computational chemistry and materials science with a Python interpreter. *Journal of Computational Chemistry*, 42 (29):2116–2129, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pecoraro:2020:SEP

[PSM+20] Adriana Pecoraro, Eduardo Schiavo, Pasqualino Maddalena, Ana B. Muñoz-García, and Michele Pavone. Structural and electronic properties of defective 2D transition metal dichalcogenide heterostructures. *Journal of Computational Chemistry*, 41(22):1946–1955, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Prasad:2021:EES

[PSMPB21] Samarjeet Prasad, Andrew C. Simmonett, Rubén Meana-Pañeda, and Bernard R. Brooks. The Extended Eighth-Shell method for periodic boundary conditions with rotational symmetry. *Journal of Computational Chemistry*, 42(19):1373–1383, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pan:2024:TML

[PSW+24] Xiaoliang Pan, Ryan Snyder, Jia-Ning Wang, Chance Lander, Carly Wickizer, Richard Van, Andrew Chesney, Yuanfei Xue, Yuezhi Mao, Ye Mei, Jingzhi Pu, and Yihan Shao. Training machine learning potentials for reactive systems: a Colab tutorial on basic models. *Journal of Computational Chemistry*, 45(10):638–647, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pant:2020:MCG

[PT20] Shashank Pant and Emad Tajkhorshid. Microscopic characterization of GRP1 PH domain interaction with anionic membranes. *Journal of Computational Chemistry*, 41(6):489–499, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Pomogaeva:2021:ISL

[PT21] Anna V. Pomogaeva and Alexey Y. Timoshkin. Influence of the solvent on the Lewis acidity of antimony pentahalides and group 13 Lewis acids toward acetonitrile and pyridine. *Journal of Computational Chemistry*, 42(25):1792–1802, September 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Parambath:2023:DQB

[PTP23] Sneha Parambath, Vishnu Thannimangalath, and Pattiyil Parameswaran. Dative quadruple bonds between d^{10} transition metals and beryllium in $BeM(PMe_3)_2$ and $BeM(CO)_2$ (M = Ni, Pd, and Pt) complexes: Transition metal fragments as six-electron donor and two-electron acceptor. *Journal of Computational Chemistry*, 44(18):1645–1652, July 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patel:2020:DBL

[PW20] Prajay Patel and Angela K. Wilson. Domain-based local pair natural orbital methods within the correlation consistent composite approach. *Journal of Computational Chemistry*, 41(8):800–813, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Patel:2020:PPL

[PWW20] Prajay Patel, Jiaqi Wang, and Angela K. Wilson. Prediction of pK_a s of late transition-metal hydrides via a QM/QM approach. *Journal of Computational Chemistry*, 41(3):171–183, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Peng:2020:APR

[PWX+20] Cheng Peng, Jinan Wang, Zhijian Xu, Tingting Cai, and Weiliang Zhu. Accurate prediction of relative binding affinities of a series of HIV-1 protease inhibitors using semi-empirical quantum mechanical charge. *Journal of Computational Chemistry*, 41(19):1773–1780, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Puzzarini:2024:IAS

[PYA24] Cristina Puzzarini, Hexu Ye, and Silvia Alessandrini. Isomerism of: Accurate structural, energetic, and spectroscopic characterization. *Journal of Computational Chemistry*, 45 (11):777–786, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Quapp:2020:SMR

[QB20] Wolfgang Quapp and Josep Maria Bofill. Some mathematical reasoning on the artificial force induced reaction method. *Journal of Computational Chemistry*, 41(7):629–634, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qi:2020:CGD

[QLC+20] Yifei Qi, Jumin Lee, Xi Cheng, Rong Shen, Shahidul M. Islam, Benoît Roux, and Wonpil Im. CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained-ensemble molecular dynamics simulations. *Journal of Computational Chemistry*, 41(5):415–420, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qian:2022:CI

[QLW+22a] Ying Qian, Xuelian Li, Jian Wu, Aimin Zhou, Zhijian Xu, and Qian Zhang. Cover image. *Journal of Computational Chem-*

istry, 43(4):i, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Qian:2022:PWO

[QLW+22b] Ying Qian, Xuelian Li, Jian Wu, Aimin Zhou, Zhijian Xu, and Qian Zhang. Picture-word order compound protein interaction: Predicting compound-protein interaction using structural images of compounds. *Journal of Computational Chemistry*, 43(4):255–264, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ravaei:2020:BDA

[RA20] Isa Ravaei and Seyed Mohammad Azami. Block deformation analysis: Density matrix blocks as intramolecular deformation density. *Journal of Computational Chemistry*, 41(29):2446–2458, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roe:2022:PAT

[RB22] Daniel R. Roe and Christina Bergonzo. `prepareforleap`: an automated tool for fast PDB-to-parameter generation. *Journal of Computational Chemistry*, 43(13):930–935, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roe:2024:MPG

[RB24] Daniel R. Roe and Bernard R. Brooks. MPI-parallelization of the grid inhomogeneous solvation theory calculation. *Journal of Computational Chemistry*, 45(10):633–637, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rappoport:2023:LMO

[RBM+23] Dmitrij Rappoport, Samuel Bekoe, Luke Nambi Mohanam, Scott Le, Naje' George, Ziyue Shen, and Filipp Furche. `Libkrylov`: a modular open-source software library for extremely large on-the-fly matrix computations. *Journal of Computational Chemistry*, 44(11):1105–1118, April 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rayon:2022:ADF

[RC22] Víctor M. Rayón and Iván Cabria. Assessment of density functional approximations for N_2 and CO_2 physisorption on benzene and graphene. *Journal of Computational Chemistry*, 43(21):1403–1419, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raucci:2020:EDB

[RCC+20] Umberto Raucci, Maria Gabriella Chiariello, Federico Coppola, Fulvio Perrella, Marika Savarese, Ilaria Ciofini, and Nadia Rega. An electron density based analysis to establish the electronic adiabaticity of proton coupled electron transfer reactions. *Journal of Computational Chemistry*, 41(20):1835–1841, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramm:2021:EMR

[RCC21] Vicente Ramm, Jehanzeb H. Chaudhry, and Christopher D. Cooper. Efficient mesh refinement for the Poisson–Boltzmann equation with boundary elements. *Journal of Computational Chemistry*, 42(12):855–869, May 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rullan:2024:MPO

[RCD+24] Raphaël Rullan, Pauline Colinet, Quentin Desdion, Stephan N. Steinmann, and Tangui Le Bahers. Modeling the polychromism of oxide minerals: The case of alexandrite and cordierite. *Journal of Computational Chemistry*, 45(12):834–842, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Roussey:2023:QQS

[RD23] Nicole M. Roussey and Alex Dickson. Quality over quantity: Sampling high probability rare events with the weighted ensemble algorithm. *Journal of Computational Chemistry*, 44(8): 935–947, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rovenchak:2024:MLA

[RD24] Andrij Rovenchak and Maksym Druchok. Machine learning-assisted search for novel coagulants: When machine learning can be efficient even if data availability is low. *Journal of Computational Chemistry*, 45(13):937–952, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rezende:2023:ABG

[RDB23] Umar Lucio Rezende, Leonardo A. De Souza, and Jadson C. Belchior. An approach based on genetic algorithms and machine learning coupled for studying alloy and molecular clusters by optimizing quantum energy surfaces. *Journal of Computational Chemistry*, 44(24):1956–1969, September 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rajasekhar:2022:INI

[RDK+22] Sreerama Rajasekhar, Soumyadip Das, Ramanathan Karuppasamy, Balamurali Musuvathi Motilal, and Kaushik Chanda. Identification of novel inhibitors for Prp protein of *Mycobacterium tuberculosis* by structure based drug design, and molecular dynamics simulations. *Journal of Computational Chemistry*, 43(9):619–630, April 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rivera:2020:FLS

[RDS+20] Miguel Rivera, Michael Dommett, Amir Sidat, Warda Rahim, and Rachel Crespo-Otero. `fromage`: A library for the study of molecular crystal excited states at the aggregate scale. *Journal of Computational Chemistry*, 41(10):1045–1058, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rapallo:2021:EDT

[RGGD21] Arnaldo Rapallo, Roberto Gaspari, Gianvito Grasso, and Andrea Danani. Extended diffusion theory: Recovering dynamics from biased/accelerated molecular simulations. *Journal of Computational Chemistry*, 42(9):586–599, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Robertson:2021:SPO

[RH21] Christopher Robertson and Scott Habershon. Simple position and orientation preconditioning scheme for minimum energy path calculations. *Journal of Computational Chemistry*, 42

(11):761–770, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rajasekhar:2021:EPI

[RKC21] Sreerama Rajasekhar, Ramanathan Karuppasamy, and Kaushik Chanda. Exploration of potential inhibitors for tuberculosis via structure-based drug design, molecular docking, and molecular dynamics simulation studies. *Journal of Computational Chemistry*, 42(24):1736–1749, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rasspe-Lange:2023:GBA

[RLHG+23] Lukas Raßpe-Lange, Alexander Hoffmann, Christoph Gertig, Joshua Heck, Kai Leonhard, and Sonja Herres-Pawlis. Geometrical benchmarking and analysis of redox potentials of copper(I/II) guanidine-quinoline complexes: Comparison of semi-empirical tight-binding and DFT methods and the challenge of describing the entatic state (part III). *Journal of Computational Chemistry*, 44(3):319–328, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Riccardi:2020:PID

[RLR+20] Enrico Riccardi, Anders Lervik, Sander Roet, Ola Aarøen, and Titus S. van Erp. PyRETIS 2: an improbability drive for rare events. *Journal of Computational Chemistry*, 41(4):370–377, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rodriguez-Mayorga:2024:ANO

[RMBSPJSG24] M. Rodríguez-Mayorga, P. Besalú-Sala, Á. J. Pérez-Jiménez, and J. C. Sancho-García. Application to nonlinear optical properties of the RSX-QIDH double-hybrid range-separated functional. *Journal of Computational Chemistry*, 45(13):995–1001, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramos:2021:DFF

[RMJ21] Chloe Ramos, Jeremiah Muehlbrad, and Benjamin G. Janesko. Density functionals with full nonlocal exchange, nonlocal rung-3.5 correlation, and D3 dispersion: Combined accuracy for general main-group thermochemistry, kinetics, and noncovalent interactions. *Journal of Computational Chemistry*, 42(27):1974–1981, October 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Reitz:2023:AOP

[RMS+23] Linda S. Reitz, Peter C. Müller, David Schnieders, Richard Dronskowski, Woon Ih Choi, Won-Joon Son, Inkook Jang, and Dae Sin Kim. On the atomistic origin of the polymorphism and the dielectric physical properties of beryllium oxide. *Journal of Computational Chemistry*, 44(10):1052–1063, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rolfes:2020:AES

[RNP20] Julian D. Rolfes, Frank Neese, and Dimitrios A. Pantazis. All-electron scalar relativistic basis sets for the elements Rb–Xe. *Journal of Computational Chemistry*, 41(20):1842–1849, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ritacca:2024:API

[RPA+24] Alessandra Gilda Ritacca, Mario Prejanò, Marta Erminia Alberto, Tiziana Marino, Marirosa Toscano, and Nino Russo. On the antibacterial photodynamic inactivation mechanism of Emodin and Dermocybin natural photosensitizers: a theoretical investigation. *Journal of Computational Chemistry*, 45(15):1254–1260, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raucci:2020:IMD

[RPD+20a] Umberto Raucci, Fulvio Perrella, Greta Donati, Maria Zoppi, Alessio Petrone, and Nadia Rega. Ab-initio molecular dynamics and hybrid explicit-implicit solvation model for aqueous and nonaqueous solvents: GFP chromophore in water and methanol solution as case study. *Journal of Computational Chemistry*, 41(26):2228–2239, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raucci:2020:CIV

[RPD+20b] Umberto Raucci, Fulvio Perrella, Greta Donati, Maria Zoppi, Alessio Petrone, and Nadia Rega. Cover image, volume 41, issue 26. *Journal of Computational Chemistry*, 41(26):C2, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Raubenolt:2022:SSP

[RR22] Bryan A. Raubenolt and Steven W. Rick. Simulation studies of polypeptoids using replica exchange with dynamical scaling and dihedral biasing. *Journal of Computational Chemistry*, 43(18):1229–1236, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ramos-Sanchez:2023:AMG

[RSHG23] Pablo Ramos-Sánchez, Jeremy N. Harvey, and José A. Gámez. An automated method for graph-based chemical space exploration and transition state finding. *Journal of Computational Chemistry*, 44(1):27–42, January 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Riccardi:2022:TIF

[RTB+22] Demian Riccardi, Zachary Trautt, Ala Bazyleva, Eugene Paulechka, Vladimir Diky, Joseph W. Magee, Andrei F. Kazakov, Scott A. Townsend, and Chris D. Muzny. Towards improved FAIRness of the ThermoML Archive. *Journal of Computational Chemistry*, 43(12):879–887, May 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rublev:2023:OED

[RTB23] Pavel Rublev, Nikolay V. Tkachenko, and Alexander I. Boldyrev. Overlapping electron density and the global delocalization of π-aromatic fragments as the reason of conductivity of the biphenylene network. *Journal of Computational Chemistry*, 44(3):168–178, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rastetter:2023:RAL

[RvWH23] Ursula Rastetter, Axel Jacobi von Wangelin, and Carmen Herrmann. Redox-active ligands as a challenge for electronic structure methods. *Journal of Computational Chemistry*, 44 (3):468–479, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Rahali:2023:HII

[RZS+23] Emna Rahali, Mohamed Oussama Zouaghi, Javier Fernandez Sanz, Noureddine Raouafi, and Youssef Arfaoui. σ-hole intermolecular interactions between carbon oxides and dihalogens: Ab-initio investigations. *Journal of Computational Chemistry*, 44(15):1426–1436, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sang-aroon:2024:CAE

[SaATR24] Wichien Sang-aroon, Marta Erminia Alberto, Marirosa Toscano, and Nino Russo. Chalcogen atom effect on the intersystem crossing kinetic constant of oxygen- and sulfur disubstituted heteroporphyrins. *Journal of Computational Chemistry*, 45(16):1322–1328, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saielli:2023:CNS

[Sai23] Giacomo Saielli. Computational NMR spectroscopy of ^{205}Tl. *Journal of Computational Chemistry*, 44(25):2016–2029, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez:2020:CIS

[Sán20] Hernán R. Sánchez. Calculation of the inner-shell contribution to the correlation energy through DLPNO-CEPA/1 and scaled same-spin second-order Møller-Plesset perturbation theory. *Journal of Computational Chemistry*, 41(10):1012–1017, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanejouand:2021:NMD

[San21] Yves-Henri Sanejouand. Normal-mode driven exploration of protein domain motions. *Journal of Computational Chemistry*, 42(31):2250–2257, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schwan:2023:IMC

[SAZ$^+$23] Sebastian Schwan, Andreas J. Achazi, Ferdinand Ziese, Peter R. Schreiner, Kerstin Volz, Stefanie Dehnen, Simone Sanna, and Doreen Mollenhauer. Insights into molecular cluster materials with adamantane-like core structures by considering dimer interactions. *Journal of Computational Chemistry*, 44(7):843–856, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stahl:2020:CAD

[SB20] Berenike Stahl and Thomas Bredow. Critical assessment of the DFT + U approach for the prediction of vanadium dioxide properties. *Journal of Computational Chemistry*, 41(3):258–265, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sorbelli:2022:ENB

[SBB+22] Diego Sorbelli, Paola Belanzoni, Leonardo Belpassi, Ji-Woong Lee, and Gianluca Ciancaleoni. An ETS-NOCV-based computational strategies for the characterization of concerted transition states involving CO_2. *Journal of Computational Chemistry*, 43(10):717–727, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schieschke:2021:GDE

[SBD+21] Nils Schieschke, Beatrix M. Bold, Philipp M. Dohmen, Daniel Wehl, Marvin Hoffmann, Andreas Dreuw, Marcus Elstner, and Sebastian Höfener. Geometry dependence of excitonic couplings and the consequences for configuration-space sampling. *Journal of Computational Chemistry*, 42(20):1402–1418, July 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salgado-Blanco:2023:EMP

[SBFSJMLU23] Daniel Salgado-Blanco, Diana S. M. Flores-Saldaña, Fabiola Jaimes-Miranda, and Florentino López-Urías. Electronic and magnetic properties of TATA-DNA sequence driven by chemical functionalization. *Journal of Computational Chemistry*, 44(12):1199–1207, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shepard:2020:RSG

[SBG20] Ron Shepard, Scott R. Brozell, and Gergely Gidofalvi. Representations of Shavitt graphs within the graphical unitary group approach. *Journal of Computational Chemistry*, 41(2):129–135, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sharma:2022:BDF

[SC22] Jyoti Sharma and Pier Alexandre Champagne. Benchmark of density functional theory methods for the study of organic polysulfides. *Journal of Computational Chemistry*, 43(32): 2131–2138, December 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schneider:2023:OSL

[SC23] Felipe S. S. Schneider and Giovanni F. Caramori. Overreact, an in silico lab: Automative quantum chemical microkinetic simulations for complex chemical reactions. *Journal of Computational Chemistry*, 44(3):209–217, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simko:2022:QCP

[SCC+22] Irén Simkó, Kalyani Chordiya, Attila G. Császár, Mousumi Upadhyay Kahaly, and Tamás Szidarovszky. A quantum-chemical perspective on the laser-induced alignment and orientation dynamics of the CH_3X (X = F, Cl, Br, I) molecules. *Journal of Computational Chemistry*, 43(8):519–538, March 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2021:EMB

[SCCZ21] Han Sun, Wei Chen, Lin Chen, and Wenqing Zheng. Exploring the molecular basis of UG-rich RNA recognition by the human splicing factor TDP-43 using molecular dynamics simulation and free energy calculation. *Journal of Computational Chemistry*, 42(23):1670–1680, September 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scheiner:2022:MOB

[Sch22a] Steve Scheiner. Maximal occupation by bases of π-hole bands surrounding linear molecules. *Journal of Computational Chemistry*, 43(5):319–330, February 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scheiner:2022:RAM

[Sch22b] Steve Scheiner. On the reliability of atoms in molecules, noncovalent index, and natural bond orbital to identify and quantify noncovalent bonds. *Journal of Computational Chemistry*, 43(26):1814–1824, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Speelman:2021:ECS

[SCKH21] Tom Speelman, Ana V. Cunha, R. K. Kathir, and Remco W. A. Havenith. Electronic couplings for singlet fission: Orbital choice and extrapolation to the complete basis set limit. *Journal of Computational Chemistry*, 42(5):326–333, February 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Search:2022:TOB

[SCvW22] Stefan D. Search, Christopher D. Cooper, and Elwin van't Wout. Towards optimal boundary integral formulations of the Poisson–Boltzmann equation for molecular electrostatics. *Journal of Computational Chemistry*, 43(10):674–691, April 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2021:REF

[SCZ+21] Tian-Yu Sun, Kai Chen, Huakang Zhou, Tingting You, Penggang Yin, and Xiao Wang. Revisiting the effect of f-functions in predicting the right reaction mechanism for hypervalent iodine reagents. *Journal of Computational Chemistry*, 42(7): 470–474, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sulka:2021:FNO

[SD21] Martin Sulka and Matús Dubecký. Fragmentation of natural orbital occupation numbers-based diagnostic of differential multireference character in complexes with hydrogen bonds. *Journal of Computational Chemistry*, 42(7):475–483, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Song:2023:CAR

[SDH23] Zilin Song, Ye Ding, and Jing Huang. Constant advance replicas method for locating minimum energy paths and transition states. *Journal of Computational Chemistry*, 44(26):2042–2057, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sadhu:2020:PTC

[SDK20] Biswajit Sadhu, Michael Dolg, and Mukund S. Kulkarni. Periodic trends and complexation chemistry of tetravalent actinide ions with a potential actinide decorporation agent 5-LIO(Me-3,2-HOPO): a relativistic density functional theory exploration. *Journal of Computational Chemistry*, 41(15): 1427–1435, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saleh:2021:NHD

[SEBE21] Marwa A. Saleh, Mohamed A. El-Badry, and Rogy R. Ezz Eldin. Novel 6-hydroxyquinolinone derivatives: Design, synthesis, antimicrobial evaluation, in silico study and toxicity profiling. *Journal of Computational Chemistry*, 42(22):1561–1578, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Siebenmorgen:2020:PPP

[SEZ20] Till Siebenmorgen, Michael Engelhard, and Martin Zacharias. Prediction of protein–protein complexes using replica exchange with repulsive scaling. *Journal of Computational Chemistry*, 41(15):1436–1447, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahoo:2024:PCS

[SFS24] Nitai P. Sahoo, Peter R. Franke, and John F. Stanton. On the performance of composite schemes in determining equilibrium molecular structures. *Journal of Computational Chemistry*, 45(16):1419–1427, June 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sikorska:2020:MLJ

[SG20] Celina Sikorska and Nicola Gaston. Modified Lennard-Jones potentials for nanoscale atoms. *Journal of Computational Chemistry*, 41(22):1985–2000, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sanchez-Gonzalez:2022:ICH

[SGGG22] Ángel Sánchez-González, Pierre Grenut, and Adrià Gil. Influence of conventional hydrogen bonds in the intercalation of phenanthroline derivatives with DNA: The important role of the sugar and phosphate backbone. *Journal of Computational Chemistry*, 43(11):804–821, April 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sachin:2024:EPO

[SGRN24] Aditya Ramesh Sachin, Gopinadhanpillai Gopakumar, Cherukuri Venkata Siva Brahmananda Rao, and Sivaraman Nagarajan. Exploring phosphoryl oxygen basicity in U(VI) complexation: a comparative study from trialkyl phosphate to phosphine oxide. *Journal of Computational Chemistry*, 45(2):70–82, January 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sagatova:2023:CSP

[SGSB23] Dinara N. Sagatova, Pavel N. Gavryushkin, Nursultan E. Sagatov, and Maksim V. Banaev. Crystal structures and P–T phase diagrams of SrC O and BaC O. *Journal of Computational Chemistry*, 44(32):2453–2460, December 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sosa:2020:ELE

[SGT+20] Akari Narayama Sosa, Israel González, Alejandro Trejo, Álvaro Miranda, Fernando Salazar, and Miguel Cruz-Irisson. Effects of lithium on the electronic properties of porous Ge as anode material for batteries. *Journal of Computational Chemistry*, 41(31):2653–2662, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sugita:2023:RSF

[SH23] Masatake Sugita and Fumio Hirata. Realization of the structural fluctuation of biomolecules in solution: Generalized Langevin mode analysis. *Journal of Computational Chemistry*, 44(10):1031–1039, April 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2023:DTHb

[SHH+23a] Yuchen Sun, Xibing He, Tingjun Hou, Lianjin Cai, Viet Hoag Man, and Junmei Wang. Development and test of highly accurate endpoint free energy methods. 1: Evaluation of ABCG2 charge model on solvation free energy prediction and optimization of atom radii suitable for more accurate solvation free energy prediction by the PBSA method. *Journal of Computational Chemistry*, 44(14):1334–1346, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2023:DTHa

[SHH+23b] Yuchen Sun, Tingjun Hou, Xibing He, Viet Hoang Man, and Junmei Wang. Development and test of highly accurate endpoint free energy methods. 2: Prediction of logarithm of n-octanol-water partition coefficient ($\log P$) for drug-like molecules using MM-PBSA method. *Journal of Computational Chemistry*, 44(13):1300–1311, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2024:PAT

[SHH+24] Ruirui Su, Xue He, K. N. Houk, Qianqian Lu, and Fang Liu. Periselectivity and ambimodal transition states in cycloadditions of tetrachloro-o-benzoquinone with 6,6-dimethylfulvene. *Journal of Computational Chemistry*, 45(11):752–760, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sulzner:2022:PAP

[SHHH22] Niklas Sülzner, Julia Haberhauer, Christof Hättig, and Arnim Hellweg. Prediction of acid pK_a values in the solvent acetone based on COSMO-RS. *Journal of Computational Chemistry*, 43(15):1011–1022, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shiga:2022:PIB

[Shi22] Motoyuki Shiga. Path integral Brownian chain molecular dynamics: a simple approximation of quantum vibrational dynamics. *Journal of Computational Chemistry*, 43(27):1864–1879, October 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stuyver:2020:TCM

[SHM+20] Thijs Stuyver, Jing Huang, Dibyendu Mallick, David Danovich, and Sason Shaik. TITAN: a code for modeling and generating electric fields-features and applications to enzymatic reactivity. *Journal of Computational Chemistry*, 41(1):74–82, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2023:RDI

[SHP+23] Xiaobo Sun, Thomas Hansen, Jordi Poater, Trevor A. Hamlin, and Friedrich Matthias Bickelhaupt. Rational design of iron catalysts for C–X bond activation. *Journal of Computational Chemistry*, 44(4):495–505, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seeger:2022:DCB

[SI22] Zoe L. Seeger and Ekaterina I. Izgorodina. A DLPNO-CCSD(T) benchmarking study of intermolecular interactions of ionic liquids. *Journal of Computational Chemistry*, 43(2): 106–120, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schaefer:2021:SCB

[SIW21] Anthony J. Schaefer, Victoria M. Ingman, and Steven E. Wheeler. SEQCROW: a ChimeraX bundle to facilitate quantum chemical applications to complex molecular systems. *Journal of Computational Chemistry*, 42(24):1750–1754, September 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Si:2024:SSC

[SJA24] Pradip Si, Ajay Jayanth, and Oliviero Andreussi. Soft-sphere continuum solvation models for nonaqueous solvents. *Journal of Computational Chemistry*, 45(11):719–737, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shen:2021:CCH

[SJZ+21] Shaojie Shen, Xinyue Jing, Xueying Zhang, Xiaoyan Li, and Yanli Zeng. The competition and cooperativity of hydrogen/halogen bond and π-hole bond involving the heteronuclear ethylene analogues. *Journal of Computational Chemistry*, 42 (13):908–916, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Smith:2020:KTR

[SK20] Cameron D. Smith and Amir Karton. Kinetics and thermodynamics of reactions involving Criegee intermediates: an assessment of density functional theory and ab initio methods through comparison with CCSDT(Q)/CBS data. *Journal of Computational Chemistry*, 41(4):328–339, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmitt:2023:TEC

[SK23] Manuel Schmitt and Ingo Krossing. Terminal end-on coordination of dinitrogen versus isoelectronic CO: a comparison using the charge displacement analysis. *Journal of Computational Chemistry*, 44(3):149–158, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See correction [Ano24a].

Somnarin:2023:CIR

[SKGG23] Thanachon Somnarin, Pacharaporn Krawmanee, Matthew Paul Gleeson, and Duangkamol Gleeson. Computational investigation of the radical-mediated mechanism of formation of difluoro methyl oxindoles: Elucidation of the reaction selectivity and yields. *Journal of Computational Chemistry*, 44(5):670–676, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sarmah:2022:HSC

[SKKG22] Kangkan Sarmah, Amlan J. Kalita, Dimpul Konwar, and Ankur K. Guha. Hydrogen storage capacity of Be_2 $(NLi)_2$ cluster with ultra-short beryllium–beryllium distance. *Journal of Computational Chemistry*, 43(26):1764–1770, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stachowicz-Kusnierz:2020:CDM

[SKKK20] Anna Stachowicz-Ku'snierz, Beata Korchowiec, and Jacek Korchowiec. Charge distributions for molecular dynamics simulations from self-consistent polarization method. *Journal of Computational Chemistry*, 41(30):2591–2597, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shekarappa:2023:DML

[SKL23] Sharath Belenahalli Shekarappa, Shivananda Kandagalla, and Julian Lee. Development of machine learning models based on molecular fingerprints for selection of small molecule inhibitors against JAK2 protein. *Journal of Computational Chemistry*, 44(16):1493–1504, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schuhmann:2021:IPM

[SKS21] Fabian Schuhmann, Vasili Korol, and Ilia A. Solov'yov. Introducing Pep McConst — a user-friendly peptide modeler for biophysical applications. *Journal of Computational Chemistry*, 42(8):572–580, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shitov:2024:MIN

[SKT24] Daniil A. Shitov, Danil V. Krutin, and Elena Yu. Tupikina. Mutual influence of non-covalent interactions formed by imidazole: a systematic quantum-chemical study. *Journal of Computational Chemistry*, 45(13):1046–1060, May 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakai:2024:LOT

[SKY24] Motoji Sakai, Mitsunori Kaneshige, and Koji Yasuda. Learning organo-transition metal catalyzed reactions by graph neural networks. *Journal of Computational Chemistry*, 45(6):341–351, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sousa:2020:ASS

[SL20] Afranio Sousa and Heveson Lima. Atomistic simulation of structural and mechanical properties of the $AMgF_3$ (A = K, Rb, and Cs) compounds under hydrostatic pressure. *Journal of Computational Chemistry*, 41(7):646–652, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Seidler:2023:BCC

[SLB23] Leopold Maximilian Seidler, Joachim Laun, and Thomas Bredow. BSSE-corrected consistent Gaussian basis sets of triple-zeta valence quality of the lanthanides La–Lu for solid-state calculations. *Journal of Computational Chemistry*, 44(15): 1418–1425, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sixto-Lopez:2021:DRT

[SLMA21] Yudibeth Sixto-López and Marlet Martínez-Archundia. Drug repositioning to target NSP15 protein on SARS-CoV-2 as possible COVID-19 treatment. *Journal of Computational Chem-*

istry, 42(13):897–907, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sun:2024:SMC

[SLML24] ChenFei Sun, Qing Liu, Lingpeng Meng, and Xiaoyan Li. Small molecules (CO_2, iPrNCO, and iPrNCN iPr) activation by the metallomimetics (μ-hydrido) diborane anion: a DFT investigation on mechanism and chemoselectivity controlling. *Journal of Computational Chemistry*, 45(6):331–340, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Savoo:2020:ASA

[SLR+20] Nandini Savoo, Jalal Z. A. Laloo, Lydia Rhyman, Ponnadurai Ramasami, F. Matthias Bickelhaupt, and Jordi Poater. Activation strain analyses of counterion and solvent effects on the ion-pair S_N2 reaction of and NH_2^- and CH_3Cl. *Journal of Computational Chemistry*, 41(4):317–327, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stuart:2020:PBW

[SM20] Duncan W. Stuart and Nicholas J. Mosey. Pseudodiagonalization-based wavefunction optimization with contracted planewave basis functions. *Journal of Computational Chemistry*, 41(3): 184–193, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Semidalas:2022:AGC

[SM22a] Emmanouil Semidalas and Jan M. L. Martin. Automatic generation of complementary auxiliary basis sets for explicitly correlated methods. *Journal of Computational Chemistry*, 43(25): 1690–1700, September 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Serdtsev:2022:ESS

[SM22b] Alexander V. Serdtsev and Nadezhda I. Medvedeva. Electronic structure, sodium diffusion and redox potentials of low-symmetry $NaMFe(MoO_4)_3$ (M = Mg, Ni). *Journal of Computational Chemistry*, 43(14):953–960, May 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Suthar:2023:OSV

[SM23] Sonam Suthar and Kartik Chandra Mondal. Open shell versus closed shell bonding interaction in cyclopropane derivatives: EDA-NOCV analyses. *Journal of Computational Chemistry*, 44(28):2184–2211, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sobhi:2023:UMR

[SMB+23] Chafia Sobhi, Lynda Merzoud, Souad Bouasla, Abdelmalek Khorief Nacereddine, Christophe Morell, and Henry Chermette. Understanding the mechanism and regio- and stereo selectivity of [3 + 2] cycloaddition reactions between substituted azomethine ylide and 3,3,3-trifluoro-1-nitroprop-1-ene, within the molecular electron density theory. *Journal of Computational Chemistry*, 44(12):1208–1220, May 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sadjadi:2021:BMG

[SMH21] SeyedAbdolreza Sadjadi, Chérif F. Matta, and Ian P. Hamilton. Bonding and metastability for Group 12 dications. *Journal of Computational Chemistry*, 42(1):40–49, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sarangi:2024:FC

[SNK24a] Ronit Sarangi, Kaushik D. Nanda, and Anna I. Krylov. Front cover. *Journal of Computational Chemistry*, 45(12):C1, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sarangi:2024:TOP

[SNK24b] Ronit Sarangi, Kaushik D. Nanda, and Anna I. Krylov. Two- and one-photon absorption spectra of aqueous thiocyanate anion highlight the role of symmetry in the condensed phase. *Journal of Computational Chemistry*, 45(12):878–885, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Segatta:2021:ISI

[SNN+21] Francesco Segatta, Artur Nenov, Daniel R. Nascimento, Niranjan Govind, Shaul Mukamel, and Marco Garavelli. iSPEC-

TRON: a simulation interface for linear and nonlinear spectra with ab-initio quantum chemistry software. *Journal of Computational Chemistry*, 42(9):644–659, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spiriti:2022:SLD

[SNW22] Justin Spiriti, Frank Noé, and Chung F. Wong. Simulation of ligand dissociation kinetics from the protein kinase PYK2. *Journal of Computational Chemistry*, 43(28):1911–1922, October 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saputri:2020:CLA

[SPSH20] Wahyu Dita Saputri, Harno Dwi Pranowo, Manuel J. Schuler, and Thomas S. Hofer. Cu^{2+} in liquid ammonia — the impact of solvent flexibility and electron correlation in ab initio quantum mechanical charge field molecular dynamics. *Journal of Computational Chemistry*, 41(25):2168–2176, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shao:2021:LCA

[SPT21] Jingjing Shao, Beate Paulus, and Jean Christophe Tremblay. Local current analysis on defective zigzag graphene nanoribbons devices for biosensor material applications. *Journal of Computational Chemistry*, 42(21):1475–1485, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schneider:2023:QCR

[SR23] Moritz Schneider and Guntram Rauhut. Quantum chemical rovibrational analysis of aminoborane and its isotopologues. *Journal of Computational Chemistry*, 44(3):298–306, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahu:2021:ICT

[SRB21] Nityananda Sahu, Jeremy O. Richardson, and Robert Berger. Instanton calculations of tunneling splittings in chiral molecules. *Journal of Computational Chemistry*, 42(4):210–221, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sahin:2020:NHM

[SS20] Kader Sahin and Emin Saripinar. A novel hybrid method named electron conformational genetic algorithm as a 4D QSAR investigation to calculate the biological activity of the tetrahydrodibenzazosines. *Journal of Computational Chemistry*, 41(11):1091–1104, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmitz:2023:ARG

[SS23] Gunnar Schmitz and Bastian Schnieder. Adaptive regularized Gaussian process regression for application in the context of hydrogen adsorption on graphene sheets. *Journal of Computational Chemistry*, 44(6):732–744, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Satyam:2024:CIE

[SS24] Jagdish Kumar Satyam and Sapan Mohan Saini. Comprehensive investigation of electronic structure, phonon spectrum and thermoelectric performance of LuMSb (M = Ni, Pd, Pt) half Heusler compounds from first principles. *Journal of Computational Chemistry*, 45(1):25–34, January 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sieradzan:2023:OPI

[SSDL+23] Adam K. Sieradzan, Jordi Sans-Duñó, Emilia A. Lubecka, Cezary Czaplewski, Agnieszka G. Lipska, Henryk Leszczyński, Krzysztof M. Ocetkiewicz, Jerzy Proficz, Paweł Czarnul, Henryk Krawczyk, and Adam Liwo. Optimization of parallel implementation of `UNRES` package for coarse-grained simulations to treat large proteins. *Journal of Computational Chemistry*, 44(4):602–625, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Solovyov:2022:CI

[SSFS22a] Ilia A. Solov'yov, Gennady Sushko, Ida Friis, and Andrey V. Solov'yov. Cover image. *Journal of Computational Chemistry*, 43(21):i, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Solovyov:2022:MMS

[SSFS22b] Ilia A. Solov'yov, Gennady Sushko, Ida Friis, and Andrey V. Solov'yov. Multiscale modeling of stochastic dynamics processes with MBN explorer. *Journal of Computational Chemistry*, 43(21):1442–1458, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sugiyama:2021:RRN

[SSM21] Kanami Sugiyama, Kenichiro Saita, and Satoshi Maeda. A reaction route network for methanol decomposition on a Pt(111) surface. *Journal of Computational Chemistry*, 42(30):2163–2169, November 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sarkar:2023:GGA

[SSMP23] Arkadeep Sarkar, Lucia Sessa, Francesco Marrafino, and Stefano Piotto. `GUIDE`: a GUI for automated quantum chemistry calculations. *Journal of Computational Chemistry*, 44(25):2030–2036, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sugiura:2020:PEC

[SSO+20] Yutaro Sugiura, Haruya Suzuki, Takuma Otomo, Takaaki Miyazaki, Toshiyuki Takayanagi, and Masanori Tachikawa. Positron–electron correlation–polarization potential model for positron binding in polyatomic molecules. *Journal of Computational Chemistry*, 41(17):1576–1585, June 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shaimardanov:2023:HAF

[SSP23] Arslan R. Shaimardanov, Dmitry A. Shulga, and Vladimir A. Palyulin. On hidden anisotropy of formally charged fragments. *Journal of Computational Chemistry*, 44(13):1312–1315, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sk:2024:MDH

[SSPK24] Md Fulbabu Sk, Sunanda Samanta, Sayan Poddar, and Parimal Kar. Microsecond dynamics of H10N7 influenza neuraminidase reveals the plasticity of loop regions and drug resistance due to the R292K mutation. *Journal of Computational Chemistry*, 45(5):247–263, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sebesta:2020:QQM

[SSS+20a] Filip Sebesta, Jakub Sebera, Vladimír Sychrovský, Yoshiyuki Tanaka, and Jaroslav V. Burda. QM and QM/MM umbrella sampling MD study of the formation of Hg(II)-thymine bond: Model for evaluation of the reaction energy profiles in solutions with constant pH. *Journal of Computational Chemistry*, 41 (16):1509–1520, June 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stylianakis:2020:BBS

[SSS+20b] Ioannis Stylianakis, Ariella Shalev, Steve Scheiner, Michael P. Sigalas, Isaiah T. Arkin, Nikolas Glykos, and Antonios Kolocouris. The balance between side-chain and backbone-driven association in folding of the α-helical influenza A transmembrane peptide. *Journal of Computational Chemistry*, 41(25): 2177–2188, September 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sabater:2023:CSE

[SSSA23] Enric Sabater, Miquel Solà, Pedro Salvador, and Diego M. Andrada. Cage-size effects on the encapsulation of P_2 by fullerenes. *Journal of Computational Chemistry*, 44(3):268–277, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Spotte-Smith:2020:ADA

[SSYB+20] Evan Walter Clark Spotte-Smith, Peiyuan Yu, Samuel M. Blau, Ravi S. Prasher, and Anubhav Jain. Aqueous Diels–Alder reactions for thermochemical storage and heat transfer fluids identified using density functional theory. *Journal of Computational Chemistry*, 41(24):2137–2150, September 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Steglenko:2020:SEO

[STB+20] Dmitriy V. Steglenko, Nikolay V. Tkachenko, Alexander I. Boldyrev, Ruslan M. Minyaev, and Vladimir I. Minkin. Stability, electronic, and optical properties of two-dimensional phosphoborane. *Journal of Computational Chemistry*, 41(15): 1456–1463, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Simm:2020:SMA

[STR20] Gregor N. Simm, Paul L. Türtscher, and Markus Reiher. Systematic microsolvation approach with a cluster-continuum scheme and conformational sampling. *Journal of Computational Chemistry*, 41(12):1144–1155, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Stsiapura:2020:SEE

[Sts20] Vitali I. Stsiapura. Solvent effect on excited state potential energy surfaces of Thioflavin T. Qualitatively different results by TDDFT and SA-2-CASSCF methods. *Journal of Computational Chemistry*, 41(21):1874–1884, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Scoditti:2021:IEL

[SVDS21] Stefano Scoditti, Vincenzo Vigna, Eslam Dabbish, and Emilia Sicilia. Iodido equatorial ligands influence on the mechanism of action of Pt(IV) and Pt(II) anti-cancer complexes: a DFT computational study. *Journal of Computational Chemistry*, 42(9):608–619, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salta:2024:NCN

[SVR$^+$24] Zoi Salta, Oscar N. Ventura, Nadjib Rais, Nicola Tasinato, and Vincenzo Barone. A new chapter in the never ending story of cycloadditions: The puzzling case of SO_2 and acetylene. *Journal of Computational Chemistry*, 45(18):1587–1602, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Salta:2022:DCT

[SVTK$^+$22] Zoi Salta, Mauricio Vega-Teijido, Aline Katz, Nicola Tasinato, Vincenzo Barone, and Oscar N. Ventura. Dipolar 1,3-cycloaddition of thioformaldehyde *S*-methylide (CH_2SCH_2) to ethylene and acetylene. A comparison with (valence) isoelectronic O_3, SO_2, CH_2OO and CH_2SO. *Journal of Computational Chemistry*, 43(21):1420–1433, August 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Safi:2021:BCP

[SW21] Zaki S. Safi and Nuha Wazzan. Benchmark calculations of proton affinity and gas-phase basicity using multilevel (G4 and G3B3), B3LYP and MP2 computational methods of para-substituted benzaldehyde compounds. *Journal of Computational Chemistry*, 42(16):1106–1117, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saito:2020:SIMa

[SWF+20] Kohei Saito, Yuya Watabe, Takashi Fujihara, Toshiyuki Takayanagi, and Jun ya Hasegawa. Spin-inversion mechanisms in O_2 binding to a model heme complex revisited by density function theory calculations. *Journal of Computational Chemistry*, 41(11):1130–1138, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shu:2022:PFI

[SWLC22] Zirui Shu, Mincong Wu, Jun Liao, and Changjun Chen. `FSATOOL 2.0`: an integrated molecular dynamics simulation and trajectory data analysis program. *Journal of Computational Chemistry*, 43(3):215–224, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saito:2020:CI

[SWM+20a] Kohei Saito, Yuya Watabe, Takaaki Miyazaki, Toshiyuki Takayanagi, and Jun ya Hasegawa. Cover image. *Journal of Computational Chemistry*, 41(29):C1, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Saito:2020:SIMb

[SWM+20b] Kohei Saito, Yuya Watabe, Takaaki Miyazaki, Toshiyuki Takayanagi, and Jun ya Hasegawa. Spin-inversion mechanisms in O_2 binding to a model heme compound: a perspective from nonadiabatic wave packet calculations. *Journal of Computational Chemistry*, 41(29):2527–2537, November 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Shimoyama:2021:ADF

[SY21] Hiromitsu Shimoyama and Yasushige Yonezawa. Atomistic detailed free-energy landscape of intrinsically disordered protein studied by multi-scale divide-and-conquer molecular dynamics simulation. *Journal of Computational Chemistry*, 42(1): 19–26, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Schmitz:2021:AWM

[SYS+21] Gunnar Schmitz, Özlem Yönder, Bastian Schnieder, Rochus Schmid, and Christof Hättig. An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. *Journal of Computational Chemistry*, 42(32):2264–2282, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Summa:2023:CFD

[SZL23] Francesco Ferdinando Summa, Riccardo Zanasi, and Paolo Lazzeretti. On the computation of frequency-dependent molecular magnetizabilities via dynamical charge and current electron densities. *Journal of Computational Chemistry*, 44 (16):1517–1530, June 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Sakae:2020:APB

[SZLD20] Yoshitake Sakae, Bin W. Zhang, Ronald M. Levy, and Nanjie Deng. Absolute protein binding free energy simulations for ligands with multiple poses, a thermodynamic path that avoids exhaustive enumeration of the poses. *Journal of Computational Chemistry*, 41(1):56–68, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Su:2020:IHH

[SZP+20] Jun Su, Tao Zhu, Thierry Pauporté, Ilaria Ciofini, and Frédéric Labat. Improving the heterointerface in hybrid organic-inorganic perovskite solar cells by surface engineering: Insights from periodic hybrid density functional theory calculations. *Journal of Computational Chemistry*, 41(19): 1740–1747, July 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tariq:2024:DIL

[TAB+24] Saad Tariq, Ayash O Alrashdi, Areej Al Bahir, S. M. Sohail Gilani, Farida Hamioud, A. A. Mubarak, Afaq Ahmed, and M. Musa Saad H.-E. DFT insights into $LaFeO_3$ with Mn substitution: a promising path to energy-efficient magneto-optical applications. *Journal of Computational Chemistry*, 45 (12):843–854, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tehrani:2023:ITA

[TAC+23] Alireza Tehrani, James S. M. Anderson, Debajit Chakraborty, Juan I. Rodriguez-Hernandez, David C. Thompson, Toon Verstraelen, Paul W. Ayers, and Farnaz Heidar-Zadeh. An information-theoretic approach to basis-set fitting of electron densities and other non-negative functions. *Journal of Computational Chemistry*, 44(25):1998–2015, September 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Taouali:2023:DFT

[TANC23] Walid Taouali, Kamel Alimi, Asma Sindhoo Nangraj, and Mark E. Casida. Density-functional theory (DFT) and time-dependent DFT study of the chemical and physical origins of key photoproperties of end-group derivatives of a nonfullerene acceptor molecule for bulk heterojunction organic solar cells. *Journal of Computational Chemistry*, 44(27):2130–2148, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tortorella:2021:CML

[TCS+21a] Sara Tortorella, Emanuele Carosati, Giulia Sorbi, Giovanni Bocci, Simon Cross, Gabriele Cruciani, and Loriano Storchi. Combining machine learning and quantum mechanics yields more chemically aware molecular descriptors for medicinal chemistry applications. *Journal of Computational Chemistry*, 42(29):2068–2078, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tortorella:2021:CI

[TCS+21b] Sara Tortorella, Emanuele Carosati, Giulia Sorbi, Giovanni Bocci, Simon Cross, Gabriele Cruciani, and Loriano Storchi. Cover image. *Journal of Computational Chemistry*, 42(29): i, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2024:ETH

[THH+24] Carson L. Tang, Alexander G. Heide, Alexandra D. Heide, Gary E. Douberly, Justin M. Turney, and Henry F. Schaefer III. Exploring the Tl H potential energy surface: a comparative analysis with group 13 systems and experiment. *Journal of Computational Chemistry*, 45(13):985–994, May 15, 2024.

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

Thomas-Hargreaves:2023:BST

[THLC+23] Lewis R. Thomas-Hargreaves, Yu-Qian Liu, Zhong-Hua Cui, Sudip Pan, and Magnus R. Buchner. Bonding situations in tricoordinated beryllium phenyl complexes. *Journal of Computational Chemistry*, 44(3):397–405, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tashiro:2021:NGO

[TIK21] Motomichi Tashiro, Yutaka Imamura, and Michio Katouda. De novo generation of optically active small organic molecules using Monte Carlo tree search combined with recurrent neural network. *Journal of Computational Chemistry*, 42(3):136–143, January 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tikhonov:2023:MSB

[Tik23] Denis S. Tikhonov. Metadynamics simulations with Bohmian-style bias potential. *Journal of Computational Chemistry*, 44 (21):1771–1775, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tolstykh:2022:UCA

[TLD+22] Daria Tolstykh, Laurent Lemmens, Stijn De Baerdemacker, Dimitri Van Neck, Patrick Bultinck, and Guillaume Acke. Uncovering Clar's aromatic π-sextet rule in the Hubbard model using Maximum Probability Domain Partitions. *Journal of Computational Chemistry*, 43(7):457–464, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tomecek:2023:ACC

[TLS23] Josef Tomecek, Cen Li, and Georg Schreckenbach. Actinium coordination chemistry: a density functional theory study with monodentate and bidentate ligands. *Journal of Computational Chemistry*, 44(3):334–345, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanida:2020:AFE

[TM20] Yoshiaki Tanida and Azuma Matsuura. Alchemical free energy calculations via metadynamics: Application to the theophylline-RNA aptamer complex. *Journal of Computational Chemistry*, 41(20):1804–1819, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tirri:2021:CMC

[TMO+21] Bernardino Tirri, Gloria Mazzone, Alistar Ottochian, Jerôme Gomar, Umberto Raucci, Carlo Adamo, and Ilaria Ciofini. A combined Monte Carlo/DFT approach to simulate UV-vis spectra of molecules and aggregates: Merocyanine dyes as a case study. *Journal of Computational Chemistry*, 42(15): 1054–1063, June 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Toutounji:2021:ESD

[Tou21] Mohamad Toutounji. Excited state distribution function for probing Herzberg–Teller vibronic coupling using linear optical response theory: Application to glassy *pheophytin a*. *Journal of Computational Chemistry*, 42(26):1905–1913, October 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Terteci-Popescu:2022:BPC

[TPB22] Andrada-Elena Terteci-Popescu and Titus Adrian Beu. Branched polyethyleneimine: CHARMM force field and molecular dynamics simulations. *Journal of Computational Chemistry*, 43(31):2072–2083, December 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tchougreeff:2021:SSQ

[TPD21] Andrei Tchougréeff, Evgeny Plekhanov, and Richard Dronskowski. Solid-state quantum chemistry with ΘΦ (ThetaPhi): Spin-liquids, superconductors, and magnetic superstructures made computationally available. *Journal of Computational Chemistry*, 42(21):1498–1513, August 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tosso:2020:CES

[TPZ+20] Rodrigo D. Tosso, Oscar Parravicini, M. Natalia C. Zarycz, Emilio Angelina, Marcela Vettorazzi, Nélida Peruchena, Sebastián Andujar, and Ricardo D. Enriz. Conformational and electronic study of dopamine interacting with the D_2 dopamine receptor. *Journal of Computational Chemistry*, 41

(21):1898–1911, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trepte:2021:PCD

[TS21] Kai Trepte and Sebastian Schwalbe. porE: a code for deterministic and systematic analyses of porosities. *Journal of Computational Chemistry*, 42(9):630–643, April 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tsuneda:2023:ROE

[TSH+23] Takao Tsuneda, Hiroki Sumitomo, Masatoshi Hasebe, Takuro Tsutsumi, and Tetsuya Taketsugu. Reactive orbital energy theory serving a theoretical foundation for the electronic theory of organic chemistry. *Journal of Computational Chemistry*, 44(2):93–104, January 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tripathy:2021:EEM

[TSR21] Vikrant Tripathy, Arjun Saha, and Krishnan Raghavachari. Electrostatically embedded molecules-in-molecules approach and its application to molecular clusters. *Journal of Computational Chemistry*, 42(10):719–734, April 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tang:2021:XFM

[TSZ+21] Zhen Tang, Yanlin Song, Shu Zhang, Wei Wang, Yuan Xu, Di Wu, Wei Wu, and Peifeng Su. XEDA, a fast and multipurpose energy decomposition analysis program. *Journal of Computational Chemistry*, 42(32):2341–2351, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tran:2020:ESN

[TT20] Van Tan Tran and Quoc Tri Tran. Electronic structures of $NbGe_n^{-/0/+}$ (n = 1—3) clusters from multiconfigurational CASPT2 and density matrix renormalization group-CASPT2 calculations. *Journal of Computational Chemistry*, 41(31): 2641–2652, December 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tupikina:2020:LPM

[TTDT20] Elena Yu. Tupikina, Konstantin G. Tokhadze, Gleb S. Denisov, and Peter M. Tolstoy. Lone pairs mapping by Laplacian of^3 He NMR chemical shift. *Journal of Computational Chemistry*, 41(12):1194–1199, May 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanimoto:2021:CMS

[TTH+21a] Shoichi Tanimoto, Koichi Tamura, Shigehiko Hayashi, Norio Yoshida, and Haruyuki Nakano. A computational method to simulate global conformational changes of proteins induced by cosolvent. *Journal of Computational Chemistry*, 42(8):552–563, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tanimoto:2021:CI

[TTH+21b] Shoichi Tanimoto, Koichi Tamura, Shigehiko Hayashi, Norio Yoshida, and Haruyuki Nakano. Cover image. *Journal of Computational Chemistry*, 42(8):C1, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Temel:2023:PAM

[TTK23] Mütesir Temel, Omer Tayfuroglu, and Abdulkadir Kocak. The performance of ANI-ML potentials for ligand–n(H_2O) interaction energies and estimation of hydration free energies from end-point MD simulations. *Journal of Computational Chemistry*, 44(4):559–569, February 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tupikina:2021:EFH

[TTT+21] Elena Yu. Tupikina, Peter M. Tolstoy, Anna A. Titova, Mikhail A. Kostin, and Gleb S. Denisov. Estimations of FH$\cdots$X hydrogen bond energies from IR intensities: Iogansen's rule revisited. *Journal of Computational Chemistry*, 42(8):564–571, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Trepte:2022:DDC

[TV22] Kai Trepte and Johannes Voss. Data-driven and constrained optimization of semi-local exchange and nonlocal correlation functionals for materials and surface chemistry. *Journal of Computational Chemistry*, 43(16):1104–1112, June 15, 2022.

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

Takaba:2022:PLB

[TWT+22] Kenichiro Takaba, Chiduru Watanabe, Atsushi Tokuhisa, Yoshinobu Akinaga, Biao Ma, Ryo Kanada, Mitsugu Araki, Yasushi Okuno, Yusuke Kawashima, Hirotomo Moriwaki, Norihito Kawashita, Teruki Honma, Kaori Fukuzawa, and Shigenori Tanaka. Protein-ligand binding affinity prediction of cyclin-dependent kinase-2 inhibitors by dynamically averaged fragment molecular orbital-based interaction energy. *Journal of Computational Chemistry*, 43(20):1362–1371, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tian:2023:PPA

[TXJT23] Hao Tian, Sian Xiao, Xi Jiang, and Peng Tao. `PASSerRank`: Prediction of allosteric sites with learning to rank. *Journal of Computational Chemistry*, 44(28):2223–2229, October 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tian:2020:MDM

[TYZ20] Jiamei Tian, Haiyan Yuan, and Jingping Zhang. Mechanistic details of metal-free cyclization reaction of organophosphorus oxide with alkynes mediated by 2,6-lutidine and Tf_2O. *Journal of Computational Chemistry*, 41(18):1709–1717, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tzeli:2021:QCB

[Tze21] Demeter Tzeli. Quadruple chemical bonding in the diatomic anions TcN^-, RuC^-, RhB^-, and $PdBe^-$. *Journal of Computational Chemistry*, 42(16):1126–1137, June 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Tosso:2022:ECS

[TZS+22] Rodrigo D. Tosso, M. Natalia C. Zarycz, Ayelén Schiel, Luisa Goicoechea Moro, Héctor A. Baldoni, Emilio Angelina, and Ricardo D. Enriz. Evaluating the conformational space of the active site of D_2 dopamine receptor. Scope and limitations of the standard docking methods. *Journal of Computa-*

tional Chemistry, 43(19):1298–1312, July 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Uddin:2023:LSP

[UAC+23] Md. Jaish Uddin, Hasina Akhter, Urmi Chowdhury, Jannatul Mawah, Sanzida Tul Karim, Mohammad Jomel, Md. Sirajul Islam, Mohammad Raqibul Islam, Latifa Afrin Bhuiyan Onin, Md. Ackas Ali, Faiyaz Md. Efaz, and Mohammad A. Halim. Large scale peptide screening against main protease of SARS CoV-2. *Journal of Computational Chemistry*, 44(8):887–901, March 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Unzueta:2020:PCM

[UB20] Pablo A. Unzueta and Gregory J. O. Beran. Polarizable continuum models provide an effective electrostatic embedding model for fragment-based chemical shift prediction in challenging systems. *Journal of Computational Chemistry*, 41(26): 2251–2265, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Usler:2023:GES

[UKBD23] Adrian L. Usler, Dennis Kemp, Alexander Bonkowski, and Roger A. De Souza. A general expression for the statistical error in a diffusion coefficient obtained from a solid-state molecular-dynamics simulation. *Journal of Computational Chemistry*, 44(14):1347–1359, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ugandi:2023:CBH

[UR23] Mihkel Ugandi and Michael Roemelt. A configuration-based heatbath-CI for spin-adapted multireference electronic structure calculations with large active spaces. *Journal of Computational Chemistry*, 44(31):2374–2390, December 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ullah:2024:BEL

[UYJ+24] Sheik Ahmed Ullah, Xin Yang, Ben Jones, Shan Zhao, Weihua Geng, and Guo-Wei Wei. Bridging Eulerian and Lagrangian Poisson–Boltzmann solvers by ESES. *Journal of Computational Chemistry*, 45(6):306–320, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vijayalakshmi:2020:ECR

[VAL20] Rajadurai Vijayalakshmi, Ramalingam Anantharaj, and Anguraj Brinda Lakshmi. Evaluation of chemical reactivity and stability of ionic liquids using ab initio and COSMO-RS model. *Journal of Computational Chemistry*, 41(9):885–912, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Verstraelen:2021:IPL

[VAP+21] Toon Verstraelen, William Adams, Leila Pujal, Alireza Tehrani, Braden D. Kelly, Luis Macaya, Fanwang Meng, Michael Richer, Raymundo Hernández-Esparza, Xiaotian Derrick Yang, Matthew Chan, Taewon David Kim, Maarten Cools-Ceuppens, Valerii Chuiko, Esteban Vöhringer-Martinez, Paul W. Ayers, and Farnaz Heidar-Zadeh. IOData: a Python library for reading, writing, and converting computational chemistry file formats and generating input files. *Journal of Computational Chemistry*, 42(6):458–464, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vassetti:2020:ACS

[VCL20] Dario Vassetti, Bartolomeo Civalleri, and Frédéric Labat. Analytical calculation of the solvent-accessible surface area and its nuclear gradients by stereographic projection: a general approach for molecules, polymers, nanotubes, helices, and surfaces. *Journal of Computational Chemistry*, 41(15):1464–1479, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valdes:2023:CCI

[VCRP23] Álvaro Valdés, Adriana Cabrera-Ramírez, and Rita Prosmiti. Confining CO_2 inside sI clathrate-hydrates: The impact of the CO_2-water interaction on quantized dynamics. *Journal of Computational Chemistry*, 44(17):1587–1598, June 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Verma:2020:MIS

[VDK+20] Neha Verma, Peter Dollinger, Filip Kovacic, Karl-Erich Jaeger, and Holger Gohlke. The membrane-integrated steric chaperone Lif facilitates active site opening of *Pseudomonas* *aeruginosa* lipase A. *Journal of Computational Chemistry*, 41 (6):500–512, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vilela:2020:PDZ

[VFCG20] Edda B. Vilela, Henrique A. Fernandes, Fábio L. Paranhos Costa, and Paulo F. Gomes. Phase diagrams of the Ziff–Gulari–Barshad model on random networks. *Journal of Computational Chemistry*, 41(22):1965–1972, August 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vijay:2024:NSB

[VHS+24] Sudarshan Vijay, Hendrik H. Heenen, Aayush R. Singh, Karen Chan, and Johannes Voss. Number of sites-based solver for determining coverages from steady-state mean-field micro-kinetic models. *Journal of Computational Chemistry*, 45(9): 546–551, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Venkatakrishnan:2024:SMO

[VKSS24] Padmavathy Venkatakrishnan, Artem V. Kuklin, Rahul Suresh, and Vijayakumar Subramaniam. Superatom molecular orbital in C_{80}. *Journal of Computational Chemistry*, 45 (12):827–833, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vassetti:2022:TTN

[VL22] Dario Vassetti and Frédéric Labat. Towards a transferable nonelectrostatic model for continuum solvation: The electrostatic and nonelectrostatic energy correction model. *Journal of Computational Chemistry*, 43(20):1372–1387, July 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Voros:2023:ESO

[VM23] Dóra Vörös and Sebastian Mai. Excited states of ortho-nitrobenzaldehyde as a challenging case for single- and multi-reference electronic structure theory. *Journal of Computational Chemistry*, 44(14):1381–1394, May 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valdes:2024:NML

[VT24] Julio J. Valdés and Alain B. Tchagang. Novel machine learning insights into the QM7b and QM9 quantum mechanics datasets. *Journal of Computational Chemistry*, 45(15):1193–1214, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valdes:2020:TSA

[VTdlM20] Esther Agacino Valdés, Gustavo Tavizón, and Pablo de la Mora. Theoretical study of Au_n clusters ($n = 1$–5) deposited on a rutile TiO_2 (110) slab, concerning structure and stability. *Journal of Computational Chemistry*, 41(32):2750–2757, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vega:2020:CI

[VV20a] Lorena Vega and Francesc Viñes. Cover image. *Journal of Computational Chemistry*, 41(30):C1, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vega:2020:GGA

[VV20b] Lorena Vega and Francesc Viñes. Generalized gradient approximation adjusted to transition metals properties: Key roles of exchange and local spin density. *Journal of Computational Chemistry*, 41(30):2598–2603, November 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vyboishchikov:2021:FNI

[VV21] Sergei F. Vyboishchikov and Alexander A. Voityuk. Fast noniterative calculation of solvation energies for water and nonaqueous solvents. *Journal of Computational Chemistry*, 42 (17):1184–1194, June 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Valencia:2021:NDG

[VWFR21] Hubert Okadome Valencia, Busheng Wang, Gilles Frapper, and Andrew Lloyd Rohl. New developments in the GDIS simulation package: Integration of VASP and USPEX. *Journal of Computational Chemistry*, 42(22):1602–1626, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vornweg:2023:SCQ

[VWJ23] Johannes R. Vornweg, Mario Wolter, and Christoph R. Jacob. A simple and consistent quantum-chemical fragmentation scheme for proteins that includes two-body contributions. *Journal of Computational Chemistry*, 44(18):1634–1644, July 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vankayala:2022:PCN

[VWP+22] Sai L. Vankayala, Luke C. Warrensford, Amanda R. Pittman, Benjamin C. Pollard, Fiona L. Kearns, Joseph D. Larkin, and H. Lee Woodcock. `CIFDock`: a novel `CHARMM`-based flexible receptor-flexible ligand docking protocol. *Journal of Computational Chemistry*, 43(2):84–95, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vyboishchikov:2023:QSE

[Vyb23] Sergei F. Vyboishchikov. A quick solvation energy estimator based on electronegativity equalization. *Journal of Computational Chemistry*, 44(3):307–318, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Vervust:2024:PCR

[VZG+24] Wouter Vervust, Daniel T. Zhang, An Ghysels, Sander Roet, Titus S. van Erp, and Enrico Riccardi. `PyRETIS 3`: Conquering rare and slow events without boundaries. *Journal of Computational Chemistry*, 45(15):1224–1234, June 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2021:RCS

[Wan21a] Yang Wang. Response to comment on “Superposition of waves or densities: Which is the nature of chemical resonance?”. *Journal of Computational Chemistry*, 42(19):1341–1343, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2021:SWD

[Wan21b] Yang Wang. Superposition of waves or densities: Which is the nature of chemical resonance? *Journal of Computational Chemistry*, 42(6):412–417, March 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2023:CGC

[Wan23] Kai Wang. $Cr_2Ge_n^-$ ($n = 15$–20) clusters with two Cr atoms exhibited antiferromagnetic coupling. *Journal of Computational Chemistry*, 44(19):1667–1672, July 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weiser:2023:SBP

[WCD+23] Jonas Weiser, Jingjing Cui, Rian D. Dewhurst, Holger Braunschweig, Bernd Engels, and Felipe Fantuzzi. Structure and bonding of proximity-enforced main-group dimers stabilized by a rigid naphthyridine diimine ligand. *Journal of Computational Chemistry*, 44(3):456–467, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2023:MBR

[WCT+23] Chao Wang, Lin Chen, Wanxia Tang, Bing Zhao, and Ruige Wang. Molecular basis of RNA recognition by TBP of HIV-1 from multiple molecular dynamics simulations and energy predictions. *Journal of Computational Chemistry*, 44(13):1291–1299, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2024:PEM

[WCY+24] Jing Wang, Sheng Chen, Qianmu Yuan, Jianwen Chen, Danping Li, Lei Wang, and Yuedong Yang. Predicting the effects of mutations on protein solubility using graph convolution network and protein language model representation. *Journal of Computational Chemistry*, 45(8):436–445, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2020:HAT

[WD20] Jun Wang and Bo Durbeej. How accurate are TD–DFT excited-state geometries compared to DFT ground-state geometries? *Journal of Computational Chemistry*, 41(18):1718–1729, July 05, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilson:2024:RCP

[WdGG24] Carter J. Wilson, Bert L. de Groot, and Vytautas Gapsys. Resolving coupled pH titrations using alchemical free energy calculations. *Journal of Computational Chemistry*, 45(17):1444–

1455, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wieder:2022:AFE

[WFBB22] Marcus Wieder, Markus Fleck, Benedict Braunsfeld, and Stefan Boresch. Alchemical free energy simulations without speed limits. a generic framework to calculate free energy differences independent of the underlying molecular dynamics program. *Journal of Computational Chemistry*, 43(17):1151–1160, June 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2023:CPL

[WFLZ23] Yu-Chen Wang, Shishi Feng, WanZhen Liang, and Yi Zhao. Comment on "A posteriori localization of many-body excited states through simultaneous diagonalization". *Journal of Computational Chemistry*, 44(27):2158–2159, October 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic). See [BMT23].

Wakchaure:2020:PBB

[WG20] Padmaja D. Wakchaure and Bishwajit Ganguly. Probing the bent bonds in cyclopropane systems for gas storage and separation process: a computational study. *Journal of Computational Chemistry*, 41(13):1271–1284, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weinhold:2021:CSW

[WG21] Frank Weinhold and Eric D. Glendening. Comment on "Superposition of Waves or Densities: Which Is the Nature of Chemical Resonance?" [J. Comput. Chem. 2021, **42**, 412–417]. *Journal of Computational Chemistry*, 42(19):1338–1340, July 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waschenbach:2020:DEG

[WGKG20] Lucas Wäschenbach, Christoph G. W. Gertzen, Verena Keitel, and Holger Gohlke. Dimerization energetics of the G-protein coupled bile acid receptor TGR5 from all-atom simulations. *Journal of Computational Chemistry*, 41(9):874–884, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Weser:2023:AHC

[WHJM23] Oskar Weser, Björn Hein-Janke, and Ricardo A. Mata. Automated handling of complex chemical structures in Z-matrix coordinates — the `chemcoord` library. *Journal of Computational Chemistry*, 44(5):710–726, February 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilson:2021:CMN

[WK21] Leighton Wilson and Robert Krasny. Comparison of the MSMS and NanoShaper molecular surface triangulation codes in the TABI Poisson–Boltzmann solver. *Journal of Computational Chemistry*, 42(22):1552–1560, August 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waite:2021:TSG

[WKCP21] Simone L. Waite, Amir Karton, Bun Chan, and Alister J. Page. Thermochemical stabilities of giant fullerenes using density functional tight binding theory and isodesmic-type reactions. *Journal of Computational Chemistry*, 42(4):222–230, February 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2021:AHP

[WKD$^+$21] Zhenghao Wu, Andreas Kalogirou, Antonio De Nicola, Giuseppe Milano, and Florian Müller-Plathe. Atomistic hybrid particle-field molecular dynamics combined with slip-springs: Restoring entangled dynamics to simulations of polymer melts. *Journal of Computational Chemistry*, 42(1):6–18, January 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2023:DKS

[WKG$^+$23] Yufeng Wu, Jiajie Kang, Wei Gao, Mingshu Bi, Dongcheng Yang, Runlai Ji, Qingwei Meng, and Cunfei Ma. A DFT and kinetic study: Is it possible to prepare epoxides without catalysts using the in-situ generated peroxy radicals or peroxides by one-step method? *Journal of Computational Chemistry*, 44(24):1917–1927, September 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wilson:2022:ARI

[WKL22] Leighton Wilson, Robert Krasny, and Tyler Luchko. Accelerating the 3D reference interaction site model theory of molecular solvation with treecode summation and cut-offs. *Journal of Computational Chemistry*, 43(18):1251–1270, July 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2023:ESE

[WLSC23a] Mincong Wu, Jun Liao, Zirui Shu, and Changjun Chen. Enhanced sampling in explicit solvent by deep learning module in FSATOOL. *Journal of Computational Chemistry*, 44(22):1845–1856, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2023:FC

[WLSC23b] Mincong Wu, Jun Liao, Zirui Shu, and Changjun Chen. Front cover. *Journal of Computational Chemistry*, 44(22):C1, August 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Walker:2022:AAP

[WLWR22] Brandon Walker, Chengwen Liu, Elizabeth Wait, and Pengyu Ren. Automation of AMOEBA polarizable force field for small molecules: Poltype 2. *Journal of Computational Chemistry*, 43 (23):1530–1542, September 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2020:MSE

[WLZM20] Jia Wang, Xiaoyan Li, Shijun Zheng, and Lingpeng Meng. Mechanism and stereoselectivity of the elementometalation process of activated alkyne $\mathrm{RC{\equiv}CR(R{=}CO_2Me)}$ by $\mathrm{Cp_2TaH_3}$. *Journal of Computational Chemistry*, 41(1):6–13, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2022:SEE

[WMJ+22] Kai Wang, Lin Miao, Zezhao Jia, Runyu Wang, Guangjia Yin, Xiaodong Zhu, Ramiro Moro, and Lei Ma. Structural evolution and electronic properties of pure and semiconductor atom doped in clusters: In_n^-, $\mathrm{In}_n\mathrm{Si}^-$, and $\mathrm{In}_n\mathrm{Ge}^-$ ($n = 3$–16). *Journal of Computational Chemistry*, 43(29):1978–1984, November

5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2020:PPC

[WMZJ20] Ting Wang, Yingjin Ma, Lian Zhao, and Jinrong Jiang. Portably parallel construction of a configuration-interaction wave function from a matrix-product state using the Charm++ framework. *Journal of Computational Chemistry*, 41(32):2707–2721, December 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Waldrop:2020:ICC

[WP20] Jonathan M. Waldrop and Konrad Patkowski. Interactions of CO_2 with cluster models of metal-organic frameworks. *Journal of Computational Chemistry*, 41(23):2066–2083, September 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Walter:2021:MML

[WRBT21] Vivien Walter, Céline Ruscher, Olivier Benzerara, and Fabrice Thalmann. `MLLPA`: a machine learning-assisted Python module to study phase-specific events in lipid membranes. *Journal of Computational Chemistry*, 42(13):930–943, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wassenaar:2022:ZST

[WRVP22] Pim N. H. Wassenaar, Emiel Rorije, Martina G. Vijver, and Willie J. G. M. Peijnenburg. ZZS similarity tool: The online tool for similarity screening to identify chemicals of potential concern. *Journal of Computational Chemistry*, 43(15): 1042–1052, June 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wei:2021:AES

[WS21] Wen-Jie Wei and Per E. M. Siegbahn. The active E4 structure of nitrogenase studied with different DFT functionals. *Journal of Computational Chemistry*, 42(2):81–85, January 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wan:2020:DCG

[WSL+20] Mingwei Wan, Junjie Song, Wenli Li, Lianghui Gao, and Weihai Fang. Development of coarse-grained force field by combining multilinear interpolation technique and simplex algorithm. *Journal of Computational Chemistry*, 41(8):814–829, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2020:LCD

[WSV20] Zhi Wang, Jessica M. J. Swanson, and Gregory A. Voth. Local conformational dynamics regulating transport properties of a Cl^- /H^+ antiporter. *Journal of Computational Chemistry*, 41 (6):513–519, March 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wada:2024:IMD

[WTST24a] Satoi Wada, Takuro Tsutsumi, Kenichiro Saita, and Tetsuya Taketsugu. Ab initio molecular dynamics study of intersystem crossing dynamics for MH_2 (M = Si, Ge, Sn, Pb) on spin-pure and spin-mixed potential energy surfaces. *Journal of Computational Chemistry*, 45(9):552–562, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wada:2024:FC

[WTST24b] Satoi Wada, Takuro Tsutsumi, Kenichiro Saita, and Tetsuya Taketsugu. Front cover. *Journal of Computational Chemistry*, 45(9):C1, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2024:MCA

[WW24] Jie Wang and Gui-Chang Wang. Mechanisms of CH_4 activation over oxygen-preadsorbed transition metals by ReaxFF and AIMD simulations. *Journal of Computational Chemistry*, 45(5):238–246, February 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2024:PPP

[WYC+24] Shuai Wang, ChiYung Yam, Shuguang Chen, LiHong Hu, Liping Li, Faan-Fung Hung, Jiaqi Fan, Chi-Ming Che, and Guan-Hua Chen. Predictions of photophysical properties of phosphorescent platinum(II) complexes based on ensemble machine learning approach. *Journal of Computational Chemistry*, 45

(6):321–330, March 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wang:2024:DSS

[WZW+24] Kai Wang, Ying Zhang, Chaoyong Wang, Jun Zhao, Le Liu, Jiaye Chen, and Yarui Wang. Discovery of a series of silicon-based ferrimagnets in $CrMnSi_n$ (n = 4–20) clusters. *Journal of Computational Chemistry*, 45(8):446–453, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Wu:2020:DOC

[WZZ+20] Zhenliang Wu, Yuwei Zhang, John Zenghui Zhang, Kelin Xia, and Fei Xia. Determining optimal coarse-grained representation for biomolecules using internal cluster validation indexes. *Journal of Computational Chemistry*, 41(1):14–20, January 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xie:2020:SMP

[XAD20] Dexuan Xie, Said H. Audi, and Ranjan K. Dash. A size-modified Poisson–Boltzmann ion channel model in a solvent of multiple ionic species: Application to voltage-dependent anion channel. *Journal of Computational Chemistry*, 41(3): 218–230, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2020:RPA

[XCJ20] Lu T. Xu, David L. Cooper, and Thom H. Dunning Jr. Resolving a puzzling anomaly in the spin-coupled generalized valence bond description of benzene. *Journal of Computational Chemistry*, 41(15):1421–1426, June 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2023:GPE

[XDZ23] Yu-Sheng Xu, Dong Die, and Ben-Xia Zheng. Growth pattern and electronic and magnetic properties of Cr-doped silver clusters. *Journal of Computational Chemistry*, 44(29):2284–2293, November 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xiao:2024:SMC

[XIV+24] Sian Xiao, Mayar Tarek Ibrahim, Gennady M. Verkhivker, Brian D. Zoltowski, and Peng Tao. β-sheets mediate the conformational change and allosteric signal transmission between the *As* LOV2 termini. *Journal of Computational Chemistry*, 45(17):1493–1504, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2022:EPH

[XLW+22] Shanshan Xu, You Li, Donghan Wang, Chao Fang, Chengwei Luo, Jiankun Deng, LiHong Hu, Hui Li, and Hongzhi Li. Efficient prediction for high precision CO-N_2 potential energy surface by stacking ensemble DNN. *Journal of Computational Chemistry*, 43(4):244–254, February 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xie:2023:KID

[XSP+23] Zhaoxuan Xie, Yinxuan Song, Fangwen Peng, Jianhao Li, Yifan Cheng, Lingzhi Zhang, Yingjin Ma, Yingqi Tian, Zhen Luo, and Haibo Ma. `Kylin 1.0`: an ab-initio density matrix renormalization group quantum chemistry program. *Journal of Computational Chemistry*, 44(13):1316–1328, May 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2020:PNS

[XZ20] Xianjin Xu and Xiaoqin Zou. PepPro: a nonredundant structure data set for benchmarking peptide-protein computational docking. *Journal of Computational Chemistry*, 41(4):362–369, February 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2024:QLM

[XZC+24] Wenjun Xu, Yanling Zhao, Jialu Chen, Zhongyu Wan, Dadong Yan, Xinghua Zhang, and Ruiqin Zhang. A Q-learning method based on coarse-to-fine potential energy surface for locating transition state and reaction pathway. *Journal of Computational Chemistry*, 45(8):487–497, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xi:2021:TDS

[XZW+21] Jinyang Xi, Liangliang Zheng, Shenghao Wang, Jiong Yang, and Wenqing Zhang. Temperature-dependent structural fluctuation and its effect on the electronic structure and charge transport in hybrid perovskite $CH_3NH_3PbI_3$. *Journal of Computational Chemistry*, 42(31):2213–2220, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xiong:2022:CBP

[XZX+22] Yuqing Xiong, Juan Zeng, Fei Xia, Qiang Cui, Xianming Deng, and Xin Xu. Conformations and binding pockets of HRas and its guanine nucleotide exchange factors complexes in the guanosine triphosphate exchange process. *Journal of Computational Chemistry*, 43(13):906–916, May 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Xu:2020:APN

[XZZ+20] Yujia Xu, Weijing Zhang, Tonglai Zhang, Wei Guo, and Yongjun Lü. Amorphous polymerization of nitrogen in compressed cupric azide. *Journal of Computational Chemistry*, 41(10):1026–1033, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshii:2020:FMM

[YAO20] Noriyuki Yoshii, Yoshimichi Andoh, and Susumu Okazaki. Fast multipole method for three-dimensional systems with periodic boundary condition in two directions. *Journal of Computational Chemistry*, 41(9):940–948, April 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2020:ODP

[YBS+20] Qingyi Yang, Woodrow Burchett, Gregory S. Steeno, Shuai Liu, Mingjun Yang, David L. Mobley, and Xinjun Hou. Optimal designs for pairwise calculation: an application to free energy perturbation in minimizing prediction variability. *Journal of Computational Chemistry*, 41(3):247–257, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yadav:2020:THN

[YC20] Sushma Yadav and Amalendu Chandra. Transport of hydrated nitrate and nitrite ions through graphene nanopores in aqueous medium. *Journal of Computational Chemistry*, 41(20):1850–1858, July 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

You:2023:EIM

[YC23] Wanli You and Yuandao Chen. Exploring the inhibition mechanism of SARS-CoV-2 main protease by ebselen: a molecular docking, molecular dynamics simulation and DFT approach. *Journal of Computational Chemistry*, 44(26):2086–2095, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2021:MEH

[YFH+21] Yongna Yuan, Shaowei Fu, Dongxu Huo, Wei Su, Ruisheng Zhang, and Jiaxuan Wei. Multipolar electrostatics for hairpin and pseudoknots in RNA: Improving the accuracy of force field potential energy function. *Journal of Computational Chemistry*, 42(11):771–786, April 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2020:PCA

[YFS20] Wenhong Yang, Timothy Tizhe Fidelis, and Wen-Hua Sun. Prediction of catalytic activities of bis(imino)pyridine metal complexes by machine learning. *Journal of Computational Chemistry*, 41(11):1064–1067, April 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yarish:2023:AMG

[YGG+23] Dzvenymyra Yarish, Sofiya Garkot, Oleksandr O. Grygorenko, Dmytro S. Radchenko, Yurii S. Moroz, and Oleksandr Gurbych. Advancing molecular graphs with descriptors for the prediction of chemical reaction yields. *Journal of Computational Chemistry*, 44(2):76–92, January 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshidome:2020:CRA

[YIO20] Takashi Yoshidome, Mitsunori Ikeguchi, and Masateru Ohta. Comprehensive 3D-RISM analysis of the hydration of small molecule binding sites in ligand-free protein structures. *Journal of Computational Chemistry*, 41(28):2406–2419, October 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2022:PIE

[YJZ+22] Xiao Yang, Mingyu Ji, Cong Zhang, Xiaoning Yang, and Zhijun Xu. Physical insight into the entropy-driven ion association. *Journal of Computational Chemistry*, 43(24):1621–1632, September 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yang:2020:EME

[YLZ+20] Sheng-Chun Yang, Bin Li, You-Liang Zhu, Aatto Laaksonen, and Yong-Lei Wang. The ENUF method — Ewald summation based on nonuniform fast Fourier transform: Implementation, parallelization, and application. *Journal of Computational Chemistry*, 41(27):2316–2335, October 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2022:CSF

[YLZ+22] Kun Yuan, Mengyang Li, Yaoxiao Zhao, Yanzhi Liu, and Xiang Zhao. Composition-selective full inclusion host-guest interaction of azobenzene-containing photoresponsive nanoring with fullerene C_{60}. *Journal of Computational Chemistry*, 43(19):1276–1285, July 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2024:SSD

[YMM+24] Isseki Yu, Takaharu Mori, Daisuke Matsuoka, Donatas Surblys, and Yuji Sugita. SPANA: Spatial decomposition analysis for cellular-scale molecular dynamics simulations. *Journal of Computational Chemistry*, 45(8):498–505, March 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yashmin:2023:CNG

[YMSS23] Farnaz Yashmin, Lakhya J. Mazumder, Rohan Sharma, and Pankaz K. Sharma. Coordination of noble gases by alkali-metal-like superatom cation Be_3B^+. *Journal of Computational Chemistry*, 44(20):1733–1739, July 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yanez:2023:DAU

[YOCMA23] Manuel Yáñez, Filiberto Ortíz-Chi, Gabriel Merino, and Ibon Alkorta. Dismantlement of ammonia upon interaction with Be_n ($n \leq 10$) clusters. *Journal of Computational Chemistry*, 44(3):159–167, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshidome:2024:FDI

[Yos24] Takashi Yoshidome. Four-dimensional imaging for cryo-electron microscopy experiments using molecular simulations and manifold learning. *Journal of Computational Chemistry*, 45(11):738–751, April 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2023:TLM

[YrYqLhC23] Rui Yu, Gai ru Yan, Yu qian Liu, and Zhong hua Cui. Two-layer molecular rotors: a zinc dimer rotating over planar hypercoordinate motifs. *Journal of Computational Chemistry*, 44(3):240–247, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yashmin:2024:NGD

[YSMS24] Farnaz Yashmin, Rohan Sharma, Lakhya J. Mazumder, and Pankaz K. Sharma. Noble gas dative bonding with coinage metal carbene complexes: a theoretical study. *Journal of Computational Chemistry*, 45(9):536–545, April 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yu:2020:DHD

[YW20] Feng Yu and Yaoting Wang. Dual-hybrid direct random phase approximation and second-order screened exchange with nonlocal van der Waals correlations for noncovalent interactions. *Journal of Computational Chemistry*, 41(10):1018–1025, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2022:PPP

[YWGY22] Lihuan Yuan, Chengkun Wu, Xiaowei Guo, and Canqun Yang. `ParaCopasi`: a package for parallel biochemical simulation and analysis. *Journal of Computational Chemistry*, 43(2):144–154, January 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Ye:2020:FBS

[YXGZ20] Linfeng Ye, Chao Xu, Feng Long Gu, and Chaoyuan Zhu. Functional and basis set dependence for time-dependent density functional theory trajectory surface hopping molecular dynamics: Cis-azobenzene photoisomerization. *Journal of Computational Chemistry*, 41(7):635–645, March 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yoshida:2020:ELS

[YYS20] Yuichiro Yoshida, Hayato Yokoi, and Hirofumi Sato. Energy landscape study of water splitting and H_2 evolution at a ruthenium(II) pincer complex. *Journal of Computational Chemistry*, 41(26):2240–2250, October 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Yuan:2021:JDF

[YYZ+21] Fang Yuan, Zhifang Yang, Xiaoying Zhang, Cuiyan Tong, Godefroid Gahungu, Wenliang Li, and Jingping Zhang. Judicious design functionalized 3D-COF to enhance CO_2 adsorption and separation. *Journal of Computational Chemistry*, 42(13):888–896, May 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zaczek:2020:MSF

[Zac20] Szymon Zaczek. MDMS: Software facilitating performing molecular dynamics simulations. *Journal of Computational Chemistry*, 41(3):266–271, January 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2023:CRD

[ZBH+23] Congcong Zhang, Han Bai, Junyuan Hu, Kai Guo, and Lili Zhao. Computationally rational design of metal-involving halogen bonds with π-covalency: Structures and bonding analysis. *Journal of Computational Chemistry*, 44(3):480–488, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2020:SNS

[ZDBZ20] Lu Zeng, Ping-Ji Deng, Jie Bi, and Ben-Chao Zhu. Searching new structures of beryllium-doped in small-sized magnesium clusters: Be_2 Mg_n^Q (q = 0, -1; n = 1-11) clusters DFT study. *Journal of Computational Chemistry*, 41(21):1885–1897, August 5, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2020:RCI

[ZFRM20] Xiaowang Zhou, Michael E. Foster, Joseph A. Ronevich, and Christopher W. San Marchi. Review and construction of interatomic potentials for molecular dynamics studies of hydrogen embrittlement in Fe-c based steels. *Journal of Computational Chemistry*, 41(13):1299–1309, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2021:REF

[ZG21] Jidong Zhang and Wei Guo. The role of electric field on decomposition of CL-20/HMX cocrystal: a reactive molecular dynamics study. *Journal of Computational Chemistry*, 42(31):2202–2212, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2020:ACC

[ZGZ+20] Daoyuan Zheng, Yurong Guo, Mingxing Zhang, Xia Feng, Lina Zhu, Lijuan Qiu, Xiaoning Jin, and Guangjiu Zhao. Anisotropic charge carrier transport of optoelectronic functional selenium-containing organic semiconductor materials. *Journal of Computational Chemistry*, 41(10):976–985, April 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2020:FUT

[ZGZC20] Haomiao Zhang, Qiankun Gong, Haozhe Zhang, and Changjun Chen. FSATOOL: a useful tool to do the conformational sampling and trajectory analysis work for biomolecules. *Journal of Computational Chemistry*, 41(2):156–164, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2024:SSF

[ZHG+24] Yueyang Zhang, Gaofeng Hu, Xueting Gao, Zhuxia Zhang, and Peng Cui. Simulation study on functional group-modified Ni-MOF-74 for CH_4 /N_2 adsorption separation. *Journal of Computational Chemistry*, 45(17):1515–1524, June 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zahn:2021:BDF

[ZHHS21] Sarah L. V. Zahn, Ole Hammerich, Poul Erik Hansen, and Stephan P. A. Sauer. The best density functional theory functional for the prediction of ^{1}H and ^{13}C chemical shifts of protonated alkylpyrroles. *Journal of Computational Chemistry*, 42(18):1248–1262, July 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2021:FEM

[ZK21] Xiaokun Zhang and James T. Kindt. Free energy of micellization of dodecyl phosphocholine (DPC) from molecular simulation: Hybrid PEACH–BAR method. *Journal of Computational Chemistry*, 42(31):2221–2232, December 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zarnecka:2023:FUF

[ZK23] Joanna M. Zarnecka and Katarzyna H. Kaminska. `FRAGMENTISE`: a user-friendly, cross-platform tool to create and analyze comprehensive small-molecule fragment databases. *Journal of Computational Chemistry*, 44(26):2096–2102, October 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhao:2023:GSA

[ZKJ+23] Mingtian Zhao, Abhishek A. Kognole, Sunhwan Jo, Aoxiang Tao, Anthony Hazel, and Alexander D. MacKerell, Jr. GPU-specific algorithms for improved solute sampling in grand canonical Monte Carlo simulations. *Journal of Computational Chemistry*, 44(20):1719–1732, July 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2022:ARM

[ZLLL22] Guan Zhang, Jin Li, Xinxin Liang, and Zongkuan Liu. Automated reaction mechanisms and kinetics with the nudged elastic band method-based AMK_Mountain and its description of the preliminary alkaline hydrolysis of nitrocellulose monomer. *Journal of Computational Chemistry*, 43(22):1513–1523, August 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2021:CPC

[ZMH+21] Na Zhang, Jinhui Mi, Suhong Huo, Lingpeng Meng, and Xiaoyan Li. Computational prediction on the catalytic activity of heterobimetallic complex featuring M–M' triple bond in acetylene cyclotrimerization: Mechanistic study. *Journal of Computational Chemistry*, 42(7):484–491, March 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhou:2022:TMP

[ZOD+22] Yingsheng Zhou, Justin M. Overhulse, Nathan J. Dupper, Yanchun Guo, Boris A. Kashemirov, Kaiyao Wei, Jérôme Govin, Carlo Petosa, and Charles E. McKenna. Toward more potent imidazopyridine inhibitors of *Candida albicans* bdf1: Modeling the role of structural waters in selective ligand binding. *Journal of Computational Chemistry*, 43(32):2121–2130, December 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2024:ALS

[ZQ24] Jin Zeng and Yue Qian. Adaptive lambda schemes for efficient relative binding free energy calculation. *Journal of Computational Chemistry*, 45(12):855–862, May 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zarate:2020:DMA

[ZRSST20] Ximena Zarate, Angela Rodriguez-Serrano, Eduardo Schott, and Jörg Tatchen. DFT/MRCI assessment of the excited-state interplay in a coumarin-schiff Mg^{2+} fluorescent sensor. *Journal of Computational Chemistry*, 41(2):136–146, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2022:RTR

[ZS22] Zheng-Feng Zhang and Ming-Der Su. The reactivity of the trapping reaction of the benzene-bridged boron/phosphorus-based frustrated Lewis pair with difluorocarbene and its group 14 analogs: a theoretical investigation. *Journal of Computational Chemistry*, 43(26):1783–1792, October 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2020:MMP

[ZSD+20] Hong Zhang, Xueguang Shao, François Dehez, Wensheng Cai, and Christophe Chipot. Modulation of membrane permeability by carbon dioxide. *Journal of Computational Chemistry*, 41(5):421–426, February 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2024:AMP

[ZWL+24a] Jia-Ming Zhang, Huai-Qian Wang, Hui-Fang Li, Xun-Jie Mei, Jin-Kun Zeng, Lan-Xin Qin, Hao Zheng, Yong-Hang Zhang, Kai-Le Jiang, Bo Zhang, and Wen-Hai Wu. Aromatic and magnetic properties in a series of heavy rare earth-doped ge_6 cluster anions. *Journal of Computational Chemistry*, 45(14): 1087–1097, May 30, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhu:2024:TIB

[ZWL24b] Zhiye Zhu, Xiaoqing Wei, and Wanzhen Liang. A theoretical investigation of benzothiadiazole derivatives for high efficiency OLEDs. *Journal of Computational Chemistry*, 45(18): 1603–1613, July 5, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2022:RCM

[ZWR22] Yi-Liang Zhang, Fu-Li Wang, and Ai-Min Ren. Reliability of computed molecular structures. *Journal of Computational Chemistry*, 43(7):465–476, March 15, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2022:TCS

[ZWY+22] Xuan Zhang, Yongtao Wang, Jia Yao, Haoran Li, and Kenji Mochizuki. A tiny charge-scaling in the OPLS-AA + L-OPLS force field delivers the realistic dynamics and structure of liquid primary alcohols. *Journal of Computational Chemistry*, 43

(6):421–430, March 5, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2020:MSIb

[ZXD20a] Hai-Feng Zheng, Jing Xu, and Yi-Hong Ding. Mono-silicon isoelectronic replacement in CAI_4: van't Hoff/Le Bel carbon or not? *Journal of Computational Chemistry*, 41(8):855, March 30, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zheng:2020:MSIa

[ZXD20b] Hai-Feng Zheng, Jing Xu, and Yi-Hong Ding. Mono-silicon isoelectronic replacement in CAl_4: van't Hoff/Le Bel carbon or not? *Journal of Computational Chemistry*, 41(2):119–128, January 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zeng:2024:SSE

[ZYZ24] Jie Zeng, Feiying You, and Jun Zhu. Screening seven-electron boron-centered radicals for dinitrogen activation. *Journal of Computational Chemistry*, 45(10):648–654, April 15, 2024. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2023:DFS

[ZZ23a] Yingfeng Zhang and Jian Zhao. A density fitting scheme for the fast evaluation of molecular electrostatic potential. *Journal of Computational Chemistry*, 44(7):806–813, March 15, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zschau:2023:MHF

[ZZ23b] Richard L. Zschau and Martin Zacharias. Mechanism of β-hairpin formation in AzoChignolin and Chignolin. *Journal of Computational Chemistry*, 44(9):988–1001, April 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Zhang:2021:RDN

[ZZG+21] Lei Zhang, Qin Zhu, Liuzhou Gao, Linlin Yang, Wei Li, Shuhua Li, Jun Zhu, Wei Wang, and Guixiang Zeng. Rational design of the nickel–borane complex for efficient hydrogenation of styrene. *Journal of Computational Chemistry*, 42(8):

545–551, March 30, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).