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

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25 May 2024
Version 1.10

Title word cross-reference

(n, n) [BW22a]. $(n \leq 10)$ [YOCMA23]. 1 [Pan23]. 16 [WMJ+22]. $1 \leq N \leq 6$ [MPOC21]. 2 [DF22, PSM+20, SLMA21]. 20 [Wan23]. 3 [TT20, WKL22]. 4 [SS20]. $4H$ [MSE+21]. 5 [AS20, JMV21, SDK20, VTdlM20]. 7 [MdSJ+23]. 8 [Bal20b]. $[3 + 2]$ [BAM+24, SMB+23]. $^{+}$ [APR21, CWZD20, GJL21, KM24, LR20, LEP+21, MAM+23, OM22, WSV20, YMSS23]. $^{-}$ [Tze21, WSV20, WMJ+22]. ^{1} [ZHHS21]. ^{13} [KWX23, MCD22, ZHHS21]. ^{19} [Ben22, MPV22]. ^{2} [AKN+20]. $^{2+}$ [ALA+22, HSG21, IK21, JRS20, MAKZ23, SPSH20, ZRSST20]. ^{205} [Sai23]. ^{3} [ERVN24, Mar21, TTDT20]. ^{31} [CMG+24, FBP+22]. $^{3}\Pi_u$ [Kop22a]. $^{3}\Sigma_g^-$ [Kop22a]. $^{\beta}$ [LL21b]. ^{I} [PAS+20]. ^{II} [ĆPP+22]. $^{\text{pro}}$ [PPP21]. ^{tz} [BVGB23]. $_{1}$ [Dor20, ERVN24]. $^{+,0,-}_{1,2,3}$ [JX24]. $_{10}$ [LR20, LXP+22]. $^{+}_{12}$ [PGP+23]. $_{18}$ [PP23]. $_{2}$ [AQRA+23, AQMM+23, AQIS+24, AMM22, ABAQ+23, AR20, AWK+23, BR23, DSC20, DBE20, DLH+23, DGSB+20, FP22, FP23, GGK20, GKA+23b,

MNH21, MML+23, MNZGO+20, MSA22b, MP23, NHFS21, OSHT20, PSM+20, RvWH23, RCC+20, SS24, SGT+20, STB+20, TPZ+20, TSH+23, UR23, VM23, WMJ+22, XZW+21, XDZ23]. **electrons** [MP23, PDGD23]. **electrooxidation** [DOT22]. **electrophilicities** [HBT+20]. **Electrophilicity** [PC23]. **electrostatic** [AS20, HS23, JGGPN21, KS24, LWLC21, LDT+22, MMK+20, ÖLP+20, UB20, VL22, ZZ23a]. **Electrostatically** [TSR21]. **Electrostatics** [HRT+20, BSB+24, SCvW22, YFH+21]. **element** [BSB+24, PLZT23]. **elementary** [DGSB+20, SYS+21]. **Elementometalation** [WLZM20]. **elements** [GPM21b, Klo22, NUK21, RCC21, RNP20]. **elimination** [KZJ21]. **Elongation** [MMK+20]. **Elucidating** [NST+20]. **Elucidation** [SKGG23, HRTSS+20]. **elusive** [DDSM23]. **embedded** [BVGB23, LLJ+24, TSR21]. **embedding** [DGSB+20, IRB+23, LWLC21, LDT+22, MMK+20, UB20]. **embrittlement** [ZFRM20]. **emission** [AS20, FB20, KBK+24]. **emitters** [LYX+22]. **Emodin** [RPA+24]. **Empirical** [LJ20, KB22, PWX+20, PNT+22, RLHG+23]. **employing** [MAI22]. **enable** [BTC24]. **enabled** [BCN22, LBH+22]. **Enabling** [ENR+24]. **Enantiomerization** [LLJ+24]. **enantiomers** [IAS+24]. **enantioselective** [IAS+24]. **enantioselectivities** [BXY+24]. **Encapsulation** [CBF+20, DSC20, SSSA23]. **Encoding** [GJMPB+20]. **End** [MXM20, Ano24a, SK23, TANC23, TTK23]. **end-group** [TANC23]. **end-on** [Ano24a, SK23]. **End-Point** [MXM20, TTK23]. **ended** [GSD+22]. **ending** [SVR+24]. **Endo** [Jab22a]. **Endo-** [Jab22a]. **endohedral** [DA22, LXP+22]. **endpoint** [SHH+23b, SHH+23a]. **ene** [SMB+23]. **energetic** [JMV21, LWC+24, PYA24]. **energetically** [NSKN21]. **Energetics** [HHL+20, NG20, NDK24, PM21, WGKG20]. **Energies** [BBK20, FMFG20, HFPS20, MFC20, NRH+20, AD23, BBY+21, BOPJ+21a, BCN22, FCB23, Fed22, GZFSM21, HCS+20, KRW+24, KPHV23, LCC+21, MPP23, MLB+23, MEKH22, MCP23, NTK21, ÖLP+20, OM22, PRF20, PFSC20, PGH24, TTK23, TTT+21, VV21]. **Energy** [FKT21, GRN20, KPR23, LPP20, MXM20, Min20, NNT+20, SZLD20, YYS20, APP24, AV20, ARR22a, AKGD24, AQRA+23, AK20, AA20, BBC20, BJ22, BBC+21a, BF22, CC22, CSGVF+20, CdSB+21, CSWW20, CSP20, DC22a, ERVN24, GH22a, GBM20, GVJ+22, HB21, HBM+20, HNCL24, HPM+21, JK21, JCMHT22, JGM21, KG23, KK23, KFTB20b, Kop22b, Kos22, LM24, LPF+23, LWF+22, LML+23, LHG+23, MML+23, MN20, MSL+20, MSA+24, MGCM21, MBBU23, NUK21, NTK21, NMFI21, NI22, NML21, OTZW24, OKI+21, PPV+21, PDC23, PCB+24, RDB23, RH21, Sán20, SSS+20a, SY21, SDH23, Sts20, SCCZ21, SHH+23b, SHH+23a, TWT+22, TSZ+21, THH+24, TM20, TAB+24, TSH+23, VL22, Vyb23, WTST24a, WCT+23, WFBB22, WdGG24, XLW+22, XZC+24, YBS+20, YFH+21, ZQ24, ZK21]. **energy-adjusted** [GH22a]. **Energy-based** [FKT21, LWF+22]. **energy-efficient** [TAB+24]. **energy-related** [CdSB+21]. **enforced** [WCD+23]. **engineering** [SZP+20]. **enhance** [YYZ+21]. **Enhanced**

DRBT24, DZL+20, DOT22, FB20, GH22a, GD23, HM21, HCS+20, HLV+24, IYI+20, IW24, KS21, KdlLC22, LRF+21, LSC24, MWK+20, MNH21, MLB+23, MFS22, MKB+21, MGCM21, MH20, MSE+21, MSS20, NEG+20, NN20, OTZW24, OE20, OMC+20, OAN+23, PCB+24, RC22, RMBSPJSG24, SDK20, dASRHB21, SC22, SSYB+20, SZP+20, TANC23, TLS23, WKCP21, ZHHS21, ZHG+24, ZGZ+20]. **functionalization** [SBFSJMLU23]. **Functionalized** [LR20, FP23, HCY+22, KGS+21, KJV23, dCB23, YYZ+21]. **functionals** [BOPJ+21a, DK23, GAP21, HMK23, HM21, HCS+20, MH22, MN20, MKK+22, NG20, RMJ21, TV22, WS21]. **Functions** [GJMPB+20, CC22, CKH23, CV22, GUCCR20, IN23b, Kop22b, MAM+23, MEKH22, MFS22, MCP23, SM20, SCZ+21, TAC+23]. **further** [BXY+24]. **fused** [BMA+24]. **fusion** [CGSP24a, EIT+21]. **future** [IRB+23]. **Fuzzy** [GJMPB+20, GJMPVR+20].

G [BWM20, CDCT21, CD20, WGKG20]. **G-protein** [WGKG20]. **G-Protein-Coupled** [BWM20]. **G3B3** [SW21]. **G4** [SW21]. **Ga** [AS20]. **GalaxyDock2** [LYKS23]. **GalaxyDock2-HEME** [LYKS23]. **gallic** [KK22a]. **GAMaterial** [LHH+23]. **gamble** [GNL+22]. **gap** [PGDD24]. **Gas** [OM23, AZKM22, APR21, DC22b, IMT+21, KGS+22, MSYS23, Mon24, MK22b, SW21, WG20, YSMS24]. **Gas-phase** [OM23, AZKM22, DC22b, IMT+21, SW21]. **gases** [YMSS23]. **Gaussian** [AAL21, BP22, GRN20, GH22b, GH23, IN23b, LB21, LB22, MP24, SS23, SLB23]. **Gaussians** [ALA20]. **GDIS** [VWFR21]. **Ge** [LXP+22, WMJ+22, Wan23, ZWL+24a, GPM21b, SGT+20, WTST24a]. **General** [Gao20, BA24, RMJ21, UKBD23, VCL20]. **general-purpose** [BA24]. **Generalized** [GCL+20, HTFY21, IWN24, SH23, VV20b, BMT+21, JKS23, LWF+22, NG20, XCJ20]. **Generalized-ensemble** [HTFY21]. **generate** [AG21]. **generated** [WKG+23]. **Generating** [SHM+20, VAP+21]. **Generation** [MC24, AMF+20, Che23, DYGM21, EVKL21, Gao20, GSD+22, JGK+22, LYX+22, Nee23, PRIP24, RB22, SM22a, dSSCC24, TIK21]. **generative** [PMT+22]. **generic** [WFBB22]. **genetic** [LHH+23, RDB23, SS20]. **genetic-algorithm** [LHH+23]. **Geometric** [ETT21b, OAC23, DHD21]. **Geometrical** [RLHG+23, GJMPVR+20, KTM+23, LWC+24]. **geometrically** [PFP+21]. **Geometries** [LXP+22, NG20, WD20]. **Geometry** [LPP20, SBD+21, AZKM22, CMD+22, LLS22a, LL21b, MMK+20, OC23]. **germa** [KDMM24]. **germaboryne** [DDSM23]. **Ge** $\equiv$ [DDSM23]. **GFN** [MKB+21, OM22]. **GFN-xTB** [MKB+21]. **GFP** [RPD+20a]. **giant** [WKCP21]. **GIAO** [MPOC21]. **GIAO-NMR** [MPOC21]. **glassy** [Tou21]. **Glioblastoma** [CM20b]. **Global** [CPG21, AZKM22, DC22a, MZ21, NAAP21, OC23, OKI+21, RTB23, TTH+21a]. **Glucopyranose** [Mon24]. **glucose** [DOT22]. **Glycans** [KUNT20]. **glycine** [HB21, ONC20]. **glycoprotein** [ONA+20]. **glycoprotein-enhanced** [ONA+20]. **glycosaminoglycan** [MGB+22]. **glycosaminoglycans** [MZMK+21]. **goal**

[LLJ+24]. **helices** [VCL20]. **helium** [BGS+20]. **Helix** [MKSS20, HTFY21, NYM22]. **helix-mimetic** [HTFY21]. **heme** [LYKS23, SWF+20, SWM+20b, LYKS23]. **hemodialysis** [MSA22a]. **hemoproteins** [FAK24]. **hepatitis** [MPuS+20]. **heptagons** [IW23]. **Herzberg** [Tou21]. **hetero** [GPM21b]. **hetero-bileptic** [GPM21b]. **heterobimetallic** [ZMH+21]. **heterocycle** [LLJ+24]. **heterocycles** [BSS+22]. **heterocyclic** [FP22, JGSA22]. **heterointerface** [SZP+20]. **heterojunction** [TANC23]. **Heterolytic** [LR20]. **heteronuclear** [KW22, SJZ+21]. **heteroporphyrins** [SaATR24]. **heterostructures** [PSM+20]. **Heusler** [SS24]. **hexa** [FDK22]. **hexa-** [FDK22]. **hexagonal** [NDK24]. **hexane** [NS22]. **Hf** [DBE20, AWK+23]. **Hg** [SSS+20a]. **hidden** [GM22, SSP23]. **Hierarchical** [NN20, dASRHB21, AÅFJ21, BTC24, LMPT21]. **High** [BLB20, EVKL21, KUNT20, LCP24, NBE+23, OKI+21, BSF20, DK23, GWN21, GVJ+22, IAF+24, KE23b, KWX23, KGG21, KDP+22, LHC+21, MZ21, PPV+21, RD23, XLW+22, ZWL24b]. **high-level** [BSF20]. **High-order** [EVKL21]. **High-performance** [BLB20]. **high-polarity** [DK23]. **high-resolution** [IAF+24]. **high-speed** [GWN21]. **High-throughput** [NBE+23]. **Higher** [HFPS20]. **highest** [KPHV23, LJW+23]. **highlight** [SNK24b]. **Highly** [JFZ+20, SHH+23b, SHH+23a]. **Hirshfeld** [LC22, MSE+21]. **histidine** [FAK24]. **histogram** [MT20b]. **HIV** [CBK+24, GG22, NPGP23, PWX+20, WCT+23]. **HIV-1** [CBK+24, PWX+20, WCT+23]. **HMX** [ZG21]. **Hoff** [ZXD20b, ZXD20a]. **Hoff/Le** [ZXD20b, ZXD20a]. **Hole** [RZS+23, JGGPN21, LK22, Sch22a, SJZ+21]. **HOMO** [CMD+22]. **HOMO-LUMO** [CMD+22]. **homodimeric** [DPSG20]. **homology** [CFOMCB+22]. **Homolytic** [LR20]. **hoops** [FDD+23]. **HOPO** [SDK20]. **Hopping** [YXGZ20, FCPG20]. **host** [BRNB21, GBM20, MJS+23, PPRS22, YLZ+22]. **host-guest** [BRNB21, GBM20, MJS+23, YLZ+22]. **hosts** [KPKS23]. **hot** [KSS21b, KSRB+21]. **HRas** [XZX+22]. **Hubbard** [POPGS22, TLD+22]. **huge** [JKK+21]. **Human** [KUNT20, KLZ+23, LSC+23, SCCZ21]. **human-norovirus** [LSC+23]. **Hybrid** [CdSB+21, ZK21, AR20, BOPJ+21a, Che23, FV20, HMK23, HUUO23, KGS+21, MN20, MKK+22, NG20, RPD+20a, RMBSPJSG24, SS20, SZP+20, WKD+21, XZW+21, YW20]. **hybrids** [CPG21, HSG21, OMC+20]. **hydrate** [MJS+23]. **hydrated** [YC20]. **hydrates** [VCRP23]. **Hydration** [ALA+22, HS22, KPTT21, PCI23, KK23, TTK23, YIO20]. **hydrazine** [PFP+21]. **hydride** [GSSG24, MC24]. **Hydrides** [PWW20]. **Hydrido** [SLML24]. **hydroalkylation** [BXY+24]. **hydrocarbon** [NS22]. **hydrocarbons** [GAP21]. **Hydrocyanation** [JFZ+20]. **Hydrogen** [AKGD24, HS23, SKKG22, AV20, ARR22b, AD23, BCN22, CVGVN+20, ĆNF23, CL23, CB20, DHN+21, DLH+23, GJL21, GH22b, KPTT21, KZ24,

[KUNT20, MBBU23, PT20, dCRM21, AR24, AA20, ASW20, BdLC21, CV22, CSWW20, COK22, GKO+22, HTTT23, HTFY21, IN23a, Jab22b, KWYN23, KLZ+23, MAM+23, MR21, MPR22, MEKH22, NI22, PHS+20, QLW+22b, SM23, TWT+22, TTK23, VCRP23, WMZJ20, WKL22, YOCMA23, YLZ+22].
interaction-site [KWYN23]. **Interactions**
[BWM20, LJ20, WP20, BW22a, BS23, BRNB21, BPDG21, CM20b, CTBB20, ERVN24, EPT21, FDD+23, FM21, HPG20, HTFY21, IL24, Klo22, KZ24, KKAK23, KGD+21, LKK+23, LEP+21, LC22, MJS+23, ODL20, OE20, PDC23, RZS+23, RMJ21, SAZ+23, SI22, SKT24, dSSCC24, YW20].
Interatomic [AA20, ZFRM20]. **intercalation** [HKSW20, SGGG22].
interest [MLGY24]. **interesting** [HPG20]. **interface**
[ABNG22, CCZ23, DMD+21, SNN+21].
interfacial [CM20a]. **intermediate**
[MMK+20].
Intermediates [SK20, DSB23, LHG+23]. **Intermolecular**
[KGD+21, OOY20, BSS+22, HTFY21, LLZ+23, MGCM21, RZS+23, SI22].
Internal [WZZ+20, ABTM22, BLB20, KZJ22]. **interoperable** [BPT+23].
Interplay [HYA+20, ZRSST20]. **Interpolation** [WSL+20, GWN21].
interpretable [BK22]. **Interpretation** [LCC+21]. **interpreter** [PSGL21].
intersection [AIV20]. **Interstitial** [PGP+21]. **intersystem**
[SaATR24, WTST24a].
intra [BOPJ+21a]. **intra-** [BOPJ+21a].
Intramolecular
[FM21, ARR22b, AIV20, CRT+21, FP22, KSP21, dCB23, RA20].
intricacies [JWS+24]. **Intrinsic** [AD20, MLGY24]. **intrinsically** [SY21]. **Introducing** [SKS21]. **invariant** [KSRB+21, OKK22]. **inverse** [LBH+22]. **inversion**
[SWF+20, SWM+20b].
Investigating [BSL20, Nan24]. **Investigation**
[CSP20, ĆPP+22, DOT22, HL20, AQMM+23, AST24, BBBP+23, DHN+21, FBM+23, KPTT21, KMR+24, KDKS21, KJV23, KK22a, MKB+21, NMMC21, RPA+24, SS20, SS24, SKGG23, SLML24, ZS22, ZWL24b].
investigations [AKGD24, BMA+24, RZS+23]. **involved** [CRT+21].
Involving [SK20, KZJ22, SJZ+21, SBB+22, ZBH+23]. **IOData** [VAP+21].
Iodido [SVDS21]. **Iodine** [ASL+20, DMTR22, SCZ+21]. **iodine-containing** [DMTR22]. **Iogansen** [TTT+21]. **Ion** [SLR+20, CX21b, FVSS20, HPG20, JRS20, LA20, OM23, dSSCC24, dSSRVdM24, XAD20, YJZ+22].
ion-induced [FVSS20]. **Ion-Pair** [SLR+20, dSSRVdM24]. **Ionic**
[VAL20, AÅFJ21, Cer22, IAS+24, LWF+22, LEP+21, SI22, XAD20].
Ionization [MLGY24, ALA20, HNCL24, MLB+23]. **ionizations** [KM24].
ions [KEK23, ODL20, SDK20, YC20]. **IR** [TTT+21, DZL+20]. **Iron**
[FAK24, CL23, GKA+23b, Jab22b, KKAK23, SHP+23].
Iron-histidine [FAK24]. **irradiation** [LYX+22]. **Irreducible** [Bal20a]. **isodesmic** [WKCP21]. **isodesmic-type** [WKCP21]. **Isoelectronic**
[ZXD20a, Ano24a, SVTK+22, SK23, ZXD20b].
isolable [FNPD22]. **isolated**
[CA22, IW23, JS21, LML+23].
Isolation [BLP20, LRKD23]. **isoleucine** [MPOC21]. **isomerase** [DPSG20]. **Isomerism** [PYA24]. **isomerization**
[GK24, OKI+21].
isomers [OKI+21, ONC20]. **isothermal** [LL21a]. **isotope**
[JMK+20, dCVARN20].
isotopologues [SR23]. **iSPECTRON** [SNN+21].

CSP20, CRT+21, DSS+24, DOT22, GPM21b, HRTSS+20, JWS+24, KZJ21, KR23, KLC+24, KSS21b, LRqG+22, LBH+22, MNH21, MIP+22, NMMC21, NST+20, PPSP20, PM21, RPA+24, SVDS21, SMB+23, SKGG23, SCZ+21, SLML24, YC23]. **mechanism-enabled** [LBH+22]. **Mechanisms** [CGMRVBAI22, WW24, BCN22, ĆNF23, LA20, LEP+21, MNZGO+20, NYM22, ONA+20, PC21, SWF+20, SWM+20b, ZLLL22]. **Mechanistic** [AMM22, BXY+24, HCY+22, JFZ+20, KZJ22, PPRS22, TYZ20, ZMH+21, ARA22, JAP+24, LGJF22]. **mechanistically** [KCF+20]. **mediate** [XIV+24]. **mediated** [JGSA22, SKGG23, TYZ20]. **medicinal** [BBB+23, TCS+21a]. **medium** [BSS+22, GH22b, GH23, LSP23, LRKD23, PDC23, YC20]. **medium-resolution** [LSP23]. **melting** [CST23]. **melts** [WKD+21]. **membered** [DSB23, KZJ22, LLJ+24]. **Membership** [GJMPB+20]. **Membrane** [BWM20, FMFG20, HHL+20, KCF+20, VDK+20, CX21b, IBL20, NLC23, ZSD+20]. **Membrane-Integrated** [VDK+20]. **Membranes** [PT20, AAID22, CBB+21, MSA22a, WRBT21]. **mer** [HHL+20, LGD+20]. **mercaptopurine** [NST+20]. **mercury** [LGD+20, MDO+20]. **Merocyanine** [TMO+21]. **mesh** [RCC21]. **mesophilic** [NYM22]. **meta** [BMT+21, NG20]. **meta-generalized** [BMT+21]. **meta-generalized-gradient** [NG20]. **metabolism** [DSS+24]. **Metadynamics** [Tik23, KN21, KSRB+21, LL21a, NN20, PPSP20, TM20]. **Metal** [HHL+20, PWW20, AR20, AS23, BKM21, DRBT24, DGM22, DOT22, ENR+24, EK20b, FBM+23, HRTSS+20, IK21, JMV21, KMR+24, MLM+24, MAM21, MAI22, MYYS24, MCD22, NBE+23, OM23, OSM20, PTP23, PDGD23, PGDD24, PSM+20, POPGS22, SKY24, TYZ20, WP20, YFS20, YMSS23, YSMS24, ZBH+23, dBCdL20, Ari24]. **metal-ammine** [MLM+24]. **metal-containing** [ENR+24]. **metal-dinitrogen** [DGM22]. **metal-doped** [DOT22]. **metal-free** [TYZ20]. **metal-involving** [ZBH+23]. **metal-ligand** [BKM21]. **metal-organic** [HRTSS+20, MAM21, WP20]. **metal-to-ligand** [IK21]. **Metal-Tren** [Ari24]. **metal/** [AR20]. **metallic** [CBF+20]. **metallo** [KGD+21]. **metallo-** [KGD+21]. **metallocenes** [HSG21]. **metallofullerenes** [DA22]. **metallomimetics** [SLML24]. **metals** [PTP23, VV20b, WW24]. **metastability** [SMH21]. **methacrylate** [MSA22a]. **methane** [DZL+20, IMT+21]. **methanol** [DHN+21, RPD+20a, SSM21]. **Method** [QB20, AD23, AKN+20, ABTM22, AYO20, AiIS+21, BBK+21, CK22, DWSX20, Dor20, EK20a, EVKL21, Fed22, Fed24, FBP+22, HKFT21, HGR+24, HTFY21, IYI+20, IN23a, IW24, JGM21, KWX23, LWF+22, LRqG+22, LC22, MMK+20, MA23a, MA23b, MT20b, MSS20, NAN+23, PDL+21, PSMPB21, RSHG23, SS20, SDH23, SKKK20, SHH+23b, SHH+23a, TTH+21a, WKG+23, XZC+24, YLZ+20, YAO20, ZK21, ZLLL22]. **method-based** [ZLLL22]. **Methods** [AWID+20, KUNT20, PAS+20, SK20, ASW20, BPT+23, BSB+24, BSF20, BF22, CTPJH22, FB21, GUCCR20, IWN24, KRSD+23, KB22, KBK+24, NBE+23, OM22, PW20, PB20, RLHG+23, RvWH23, SW21, SYS+21, SM22a, SC22, Sts20, SHH+23b, SHH+23a, TZS+22]. **methotrexate** [PRH20].

GJMPVR+20, GK24, GG22, GSJ+23, HS23, HGF20, HPM+21, IAS+24, JKK+21, KZJ21, KG23, KK23, KI24, KLP+22, KTBS23, KPHV23, KS24, KGD+21, LL21a, LKM20, LHH+21, LKK+23, LKT21, LCLB24, LEP+21, LAM+23, MP24, MN20, MKK+22, MGB+22, MSA+24, MK22a, MAP+20, NAN+23, NI22, NGD22, NN20, NP23, OSHT20, PBM21, PDL+21].
molecular
[POvG21, PPP21, PL22, PSB+22, PM21, QLC+20, RKC21, RDK+22, RGGD21, RPD+20a, RDB23, RDS+20, SFS24, SPSH20, SIW21, SYS+21, SAZ+23, SCvW22, SKL23, Shi22, SY21, SWLC22, SMB+23, SKKK20, SZL23, SCCZ21, TWT+22, TPB22, TCS+21a, TSR21, UKBD23, VKSS24, WTST24a, WFBB22, WK21, WKL22, WKD+21, YGG+23, Yos24, YC23, YrYqLhC23, YMM+24, ZK21, ZG21, ZWR22, ZZ23a, ZFRM20, KZJ22].
molecular-dynamics [UKBD23]. **molecular-orbital** [KK23].
molecular-wide [BdLC21]. **molecule** [AK20, BBBP+23, GFRNC21, KDMM24, KFTB20b, MC24, Mon24, Ore24, SKL23, TANC23, YIO20, ZK23].
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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).

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[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).

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[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

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[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).

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[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).

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[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).

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[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).

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

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[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).

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[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).

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[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-*

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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 do-

main 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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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

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[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).

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[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).

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[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).

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[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).

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[SC22] Jyoti Sharma and Pier Alexandre Champagne. Benchmark of density functional theory methods for the study of organic

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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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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 ac-

tinide 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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[SLB23] Leopold Maximilian Seidler, Joachim Laun, and Thomas Bredow. BSSE-corrected consistent Gaussian basis sets of triplezeta 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).

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[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, *i*PrNCO, and *i*PrNCN *i*Pr) 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).

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[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).

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[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).

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[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).

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[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).

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[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).

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[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 pro-

cesses 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).

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[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).

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[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).

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