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

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Anisimov:2020:IEC

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Anonymous:2020:IIo

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Anonymous:2020:IIu

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Anonymous:2020:IIw

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Anonymous:2020:IIbe

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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

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Anonymous:2021:IIb

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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

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[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:IIaa

[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).

Arrue:2021:SCB

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

Ahn:2020:PWA

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

Al-Qaisi:2023:TIL

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

Ananthaneni:2020:CST

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

Abdullayev:2022:CMS

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

Afonin:2022:GTC

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

Afonin:2022:MTA

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

Anjali:2020:AEP

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

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

Anila:2023:FMS

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

Alberto:2020:ISP

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

Aquino:2020:FON

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

Afonin:2020:QDR

[AV20] Andrei V. Afonin and Alexander V. Vashchenko. Quantitative decomposition of resonance-assisted hydrogen bond energy in β-diketones into resonance and hydrogen bonding (π- and σ-) components using molecular tailoring and function-based approaches. *Journal of Computational Chemistry*, 41(13):1285–1298, May 15, 2020. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Arroyuelo:2021:EQP

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

Awoonor-Williams:2020:QCM

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

Anders:2023:CBH

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

Andoh:2020:EFM

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

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

Bae:2022:TDD

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

Beu:2020:MFF

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

Balasubramanian:2020:CCH

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

Balasubramanian:2020:NWO

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

Banavali:2020:MCM

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

Bekker:2020:ESC

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

Brodney:2023:IDE

[BBB+23] Marian D. Brodney, Gregory Bakken, Christopher R. Butler, Jacquelyn Klug-McLeod, Robert Owen, and Shao-Tien Sng. Integrated design environment: a multi-use platform for design idea capture, evaluation, and tracking in medicinal chemistry. *Journal of Computational Chemistry*, 44(6):

788–800, March 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

Banik:2020:QMS

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

Blasiak:2021:IEO

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

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

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

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

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

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[BHR$^+$21] Ridha Ben Said, Riadh Hanachi, Seyfeddine Rahali, Mohammed A. M. Alkhalifah, Faisal Alresheedi, Bahoueddine Tangour, and Majdi Hochlaf. Evaluation of a new series of pyrazole derivatives as a potent epidermal growth factor receptor inhibitory activity: QSAR modeling using quantum-chemical descriptors. *Journal of Computational Chemistry*, 42(32):2306–2320, December 15, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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

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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).

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[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].

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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).

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[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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[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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[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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[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 domain in dimerization of amyloid precursor protein. *Journal of Computational Chemistry*, 44(15):1437–1445, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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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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[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,

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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).

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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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[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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[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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[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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[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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[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).

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[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).

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[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

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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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[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].

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

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

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

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

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

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

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Mahajan:2020:EMC

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[RZS+23] Emna Rahali, Mohamed Oussama Zouaghi, Javier Fernandez Sanz, Noureddine Raouafi, and Youssef Arfaoui. σ-hole intermolecular interactions between carbon oxides and dihalogens: Ab-initio investigations. *Journal of Computational Chemistry*, 44(15):1426–1436, June 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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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 Chemistry*, 42(13):897–907, May 15, 2021. 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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[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).

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[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).

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[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).

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[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).

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[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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[SSSA23] Enric Sabater, Miquel Solà, Pedro Salvador, and Diego M. Andrada. Cage-size effects on the encapsulation of P_2 by fullerenes. *Journal of Computational Chemistry*, 44(3):268–277, January 30, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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[SWLC22] Zirui Shu, Mincong Wu, Jun Liao, and Changjun Chen. `FSATOOL 2.0`: an integrated molecular dynamics simulation and trajectory data analysis program. *Journal of Computational Chemistry*, 43(3):215–224, January 30, 2022. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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[TCS+21b] Sara Tortorella, Emanuele Carosati, Giulia Sorbi, Giovanni Bocci, Simon Cross, Gabriele Cruciani, and Loriano Storchi. Cover image. *Journal of Computational Chemistry*, 42(29): i, November 5, 2021. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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[Tik23] Denis S. Tikhonov. Metadynamics simulations with Bohmian-style bias potential. *Journal of Computational Chemistry*, 44 (21):1771–1775, August 5, 2023. CODEN JCCHDD. ISSN 0192-8651 (print), 1096-987X (electronic).

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