A Complete Bibliography of Publications in *The International Journal of Quantum Chemistry*: 2020–2029

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

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

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

08 November 2023
Version 1.08

Title word cross-reference

References

Amini:2020:ADD

[AA20] Samad Amini and Seyed Mohammad Azami. Asymmetric deformation density analysis in carbon nanotubes. *International Journal of Quantum Chemistry*, 120(17):e26277:1–e26277:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdelhadi:2022:MSZ

[AAB22] Sofiane Abdelhadi, Hamza Abid, and Djillali Bensaid. Mg substitution in zinc selenide: Enhanced optoelectronic and thermoelectric performance. *International Journal of Quantum Chemistry*, 122(10):e26883:1–e26883:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2020:TSS

[AAM+20] Malak Azmat Ali, Neda Alam, Meena, Sonbal Ali, Sajad Ahmad Dar, Afzal Khan, G. Murtaza, and A. Laref. A theoretical study of the structural, thermoelectric, and spin–orbit coupling influenced optoelectronic properties of $CsTmCl_3$ halide perovskite. *International Journal of Quantum Chemistry*, 120(7):e26141:1–e26141:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdullayev:2021:CMS

[AAN+21] Yusif Abdullayev, Vagif Abbasov, Fuzuli Nasirov, Nigar Rzayeva, Leyla Nasibova, and Jochen Autschbach. Computational mechanistic studies of the carbon–carbon double bond difunctionalization via epoxidation and subsequent aminolysis in vegetable oils. *International Journal of Quantum Chemistry*, 121(10):e26609:1–e26609:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Araujo:2021:CRA

[AB21] Judith P. Araújo and Maikel Y. Ballester. A comparative review of 50 analytical representation of potential energy interaction for diatomic systems: 100 years of history. *International Journal of Quantum Chemistry*, 121(24):e26808:1–e26808:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ash:2022:CIM

[ABDD22] Tamalika Ash, Soumadip Banerjee, Tanay Debnath, and Abhijit K. Das. Computational insights into the multi-Diels–Alder reactions of neutral C_{60} and its Li^+ encapsulated analogue: a density functional theory study. *International Journal of Quantum Chemistry*, 122(2):e26824:1–e26824:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alenaizan:2020:PIR

[ABS20] Asem Alenaizan, Lori A. Burns, and C. David Sherrill. Python implementation of the restrained electrostatic potential charge model. *International Journal of Quantum Chemistry*, 120(2):e26035:1–e26035:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ashhab:2020:OGS

[ACM20] Sahel Ashhab, Marcelo Carignano, and Mohamed E. Madjet. Order in the ground state of a simple cubic dipole lattice in an external field. *International Journal of Quantum Chemistry*, 120(1):e26053:1–e26053:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azari:2022:MPE

[AD22] Mahdieh Azari and Nasrin Dehgardi. Measuring peripherality extent in chemical graphs via graph operations. *International Journal of Quantum Chemistry*, 122(3):e26835:1–e26835:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2021:SMW

[ADZA21] Akbar Ali, Zhibin Du, Syeda Sifwa Zaineb, and Tariq Alraqad. On the second maximum Wiener polarity index of chemical trees of a fixed order. *International Journal of Quantum Chemistry*, 121(11):e26631:1–e26631:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akhter:2021:CMI

[AIAG21] Shehnaz Akhter, Zahid Iqbal, Adnan Aslam, and Wei Gao. Computation of Mostar index for some graph operations. *International Journal of Quantum Chemistry*, 121 (15):e26674:1–e26674:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Altun:2021:LED

[AIB21] Ahmet Altun, Róbert Izsák, and Giovanni Bistoni. Local energy decomposition of coupled-cluster interaction energies: Interpretation, benchmarks, and comparison with symmetry-adapted perturbation theory. *International Journal of Quantum Chemistry*, 121(3):e26339:1–e26339:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akhter:2021:MIS

[AII21] Shehnaz Akhter, Muhammad Imran, and Zahid Iqbal. Mostar indices of SiO_2 nanostructures and melem chain nanostructures. *International Journal of Quantum Chemistry*, 121(5):e26520:1–e26520:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amadi:2020:SEF

[AIN$^+$20] Precious O. Amadi, Akpan N. Ikot, Alalibo T. Ngiangia, Uduakobong S. Okorie, Gaotsiwe J. Rampho, and Hewa Y. Abdullah. Shannon entropy and Fisher information for screened Kratzer potential. *International Journal of Quantum Chemistry*, 120(14):e26246:1–e26246:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aireti:2021:CLS

[AJC$^+$21] Maidina Aireti, Yi Jiang, Haibin Cao, Haiming Duan, Xiuhua Cui, Qun Jing, and Xun Xue. The cage-like structure enhanced magnetic moment in ScK_n (n = 2–12) clusters: a first-principles jointed particle swarm optimization investigation. *International Journal of Quantum Chemistry*, 121 (14):e26654:1–e26654:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdel-khalek:2021:AFI

[AkAR+21] S. Abdel-khalek, Azhri Alhag, Mahmoud Ragab, S. M. Abo-Dahab, Ali Algarni, and Hijaz Ahmad. Atomic Fisher information and entanglement forecasting for quantum system based on artificial neural network and time series model. *International Journal of Quantum Chemistry*, 121(4):e26446:1–e26446:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arockiaraj:2021:RSC

[AKK+21] Micheal Arockiaraj, Sandi Klavzar, S. Ruth Julie Kavitha, Shagufa Mushtaq, and Krishnan Balasubramanian. Relativistic structural characterization of molybdenum and tungsten disulfide materials. *International Journal of Quantum Chemistry*, 121(5):e26492:1–e26492:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2020:CPM

[AKKN20] Sajjad Ali, Muhammad Baber Azam Khan, Said Alam Khan, and Noora. The catalytic performance of metal-free defected carbon catalyst towards acetylene hydrochlorination revealed from first-principles calculation. *International Journal of Quantum Chemistry*, 120(24):e26418:1–e26418:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aulicino:2022:SPE

[AKP22] Joseph C. Aulicino, Trevor Keen, and Bo Peng. State preparation and evolution in quantum computing: a perspective from Hamiltonian moments. *International Journal of Quantum Chemistry*, 122(5):e26853:1–e26853:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2020:RTI

[Ali20] Akbar Ali. Remarks on topological indices of carbon nanocones and nanotori. *International Journal of Quantum Chemistry*, 120(17):e26331:1–e26331:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2020:MPF

[AMK+20] Malak Azmat Ali, G. Murtaza, Afzal Khan, Eman Algrafy, Asif Mahmood, and Shahid M. Ramay. Magneto-electronic properties of ferromagnetic compounds Rb_2TaZ_6 (Z = Cl, Br) for possible spintronic applications. *International Journal of Quantum Chemistry*, 120(19):e26357:1–e26357:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aucar:2021:RCE

[AMM21] Juan J. Aucar, Alejandro F. Maldonado, and Juan I. Melo. Relativistic corrections of the electric field gradient in dihalogen molecules XY (X, Y = F, Cl, Br, I, At) within the linear response elimination of the small component formalism. *International Journal of Quantum Chemistry*, 121(20): e26769:1–e26769:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdeveiszadeh:2020:TIS

[AN20] Zeinab Abdeveiszadeh and Siamak Noorizadeh. Theoretical investigation on the structure and stability of some neutral noble gas compounds containing Xe–Xe bond. *International Journal of Quantum Chemistry*, 120(11):e26185:1–e26185:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVa

[Ano20a] Anonymous. Cover image, volume 120, issue 1. *International Journal of Quantum Chemistry*, 120(1):e26098:1–e26098:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVj

[Ano20b] Anonymous. Cover image, volume 120, issue 10. *International Journal of Quantum Chemistry*, 120(10):e26224:1–e26224:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVk

[Ano20c] Anonymous. Cover image, volume 120, issue 11. *International Journal of Quantum Chemistry*, 120(11):e26240:1–

e26240:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVl

[Ano20d] Anonymous. Cover image, volume 120, issue 12. *International Journal of Quantum Chemistry*, 120(12):e26241:1–e26241:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVm

[Ano20e] Anonymous. Cover image, volume 120, issue 13. *International Journal of Quantum Chemistry*, 120(13):e26272:1–e26272:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVn

[Ano20f] Anonymous. Cover image, volume 120, issue 14. *International Journal of Quantum Chemistry*, 120(14):e26337:1–e26337:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVo

[Ano20g] Anonymous. Cover image, volume 120, issue 15. *International Journal of Quantum Chemistry*, 120(15):e26345:1–e26345:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVp

[Ano20h] Anonymous. Cover image, volume 120, issue 16. *International Journal of Quantum Chemistry*, 120(16):e26384:1–e26384:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVq

[Ano20i] Anonymous. Cover image, volume 120, issue 17. *International Journal of Quantum Chemistry*, 120(17):e26395:1–e26395:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVr

[Ano20j] Anonymous. Cover image, volume 120, issue 18. *International Journal of Quantum Chemistry*, 120(18):e26420:1–

e26420:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVs

[Ano20k] Anonymous. Cover image, volume 120, issue 19. *International Journal of Quantum Chemistry*, 120(19):e26465:1–e26465:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVb

[Ano20l] Anonymous. Cover image, volume 120, issue 2. *International Journal of Quantum Chemistry*, 120(2):e26125:1–e26125:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVt

[Ano20m] Anonymous. Cover image, volume 120, issue 20. *International Journal of Quantum Chemistry*, 120(20):e26484:1–e26484:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVu

[Ano20n] Anonymous. Cover image, volume 120, issue 22. *International Journal of Quantum Chemistry*, 120(22):e26505:1–e26505:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVv

[Ano20o] Anonymous. Cover image, volume 120, issue 24. *International Journal of Quantum Chemistry*, 120(24):e26539:1–e26539:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVc

[Ano20p] Anonymous. Cover image, volume 120, issue 3. *International Journal of Quantum Chemistry*, 120(3):e26138:1–e26138:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVd

[Ano20q] Anonymous. Cover image, volume 120, issue 4. *International Journal of Quantum Chemistry*, 120(4):e26156:1–e26156:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVe

[Ano20r] Anonymous. Cover image, volume 120, issue 5. *International Journal of Quantum Chemistry*, 120(5):e26164:1–e26164:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVf

[Ano20s] Anonymous. Cover image, volume 120, issue 6. *International Journal of Quantum Chemistry*, 120(6):e26173:1–e26173:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVg

[Ano20t] Anonymous. Cover image, volume 120, issue 7. *International Journal of Quantum Chemistry*, 120(7):e26177:1–e26177:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVh

[Ano20u] Anonymous. Cover image, volume 120, issue 8. *International Journal of Quantum Chemistry*, 120(8):e26199:1–e26199:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:CIVi

[Ano20v] Anonymous. Cover image, volume 120, issue 9. *International Journal of Quantum Chemistry*, 120(9):e26205:1–e26205:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIa

[Ano20w] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(1):e26099:1–e26099:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIb

[Ano20x] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(2):e26126:1–e26126:??, January

15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIc

[Ano20y] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(3):e26139:1–e26139:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IId

[Ano20z] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(4):e26157:1–e26157:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIe

[Ano20-27] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(5):e26163:1–e26163:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIf

[Ano20-28] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(6):e26174:1–e26174:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIg

[Ano20-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(7):e26178:1–e26178:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIh

[Ano20-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(8):e26200:1–e26200:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIi

[Ano20-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(9):e26206:1–e26206:??, May 5,

2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIj

[Ano20-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(10):e26227:1–e26227:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIk

[Ano20-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(11):e26242:1–e26242:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIl

[Ano20-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(12):e26271:1–e26271:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIm

[Ano20-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(13):e26273:1–e26273:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIn

[Ano20-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(14):e26338:1–e26338:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIo

[Ano20-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(15):e26346:1–e26346:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIp

[Ano20-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(16):e26385:1–e26385:??, August

15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIq

[Ano20-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(17):e26396:1–e26396:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIr

[Ano20-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(18):e26421:1–e26421:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIs

[Ano20-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(19):e26466:1–e26466:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIt

[Ano20-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(20):e26485:1–e26485:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIu

[Ano20-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(21):e26497:1–e26497:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIv

[Ano20-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(22):e26506:1–e26506:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIw

[Ano20-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(23):e26514:1–e26514:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:IIx

[Ano20-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 120(24):e26540:1–e26540:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2020:SIM

[Ano20-47] Anonymous. Special issue on MERCURY. *International Journal of Quantum Chemistry*, 120(20):e26481:1–e26481:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:C

[Ano21a] Anonymous. Corrigendum. *International Journal of Quantum Chemistry*, 121(23):e26801:1–e26801:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVa

[Ano21b] Anonymous. Cover image, volume 121, issue 1. *International Journal of Quantum Chemistry*, 121(1):e26280:1–e26280:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVf

[Ano21c] Anonymous. Cover image, volume 121, issue 10. *International Journal of Quantum Chemistry*, 121(10):e26298:1–e26298:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVg

[Ano21d] Anonymous. Cover image, volume 121, issue 11. *International Journal of Quantum Chemistry*, 121(11):e26300:1–e26300:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVh

[Ano21e] Anonymous. Cover image, volume 121, issue 12. *International Journal of Quantum Chemistry*, 121(12):e26302:1–

e26302:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVi

[Ano21f] Anonymous. Cover image, volume 121, issue 13. *International Journal of Quantum Chemistry*, 121(13):e26304:1–e26304:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVj

[Ano21g] Anonymous. Cover image, volume 121, issue 15. *International Journal of Quantum Chemistry*, 121(15):e26308:1–e26308:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVk

[Ano21h] Anonymous. Cover image, volume 121, issue 16. *International Journal of Quantum Chemistry*, 121(16):e26310:1–e26310:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVm

[Ano21i] Anonymous. Cover image, volume 121, issue 17. *International Journal of Quantum Chemistry*, 121(17):e26312:1–e26312:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVn

[Ano21j] Anonymous. Cover image, volume 121, issue 18. *International Journal of Quantum Chemistry*, 121(18):e26314:1–e26314:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVo

[Ano21k] Anonymous. Cover image, volume 121, issue 19. *International Journal of Quantum Chemistry*, 121(19):e26316:1–e26316:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVp

[Ano21l] Anonymous. Cover image, volume 121, issue 20. *International Journal of Quantum Chemistry*, 121(20):e26318:1–

e26318:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVq

[Ano21m] Anonymous. Cover image, volume 121, issue 21. *International Journal of Quantum Chemistry*, 121(21):e26320:1–e26320:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVr

[Ano21n] Anonymous. Cover image, volume 121, issue 22. *International Journal of Quantum Chemistry*, 121(22):e26322:1–e26322:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVs

[Ano21o] Anonymous. Cover image, volume 121, issue 23. *International Journal of Quantum Chemistry*, 121(23):e26324:1–e26324:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVt

[Ano21p] Anonymous. Cover image, volume 121, issue 24. *International Journal of Quantum Chemistry*, 121(24):e26326:1–e26326:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVb

[Ano21q] Anonymous. Cover image, volume 121, issue 6. *International Journal of Quantum Chemistry*, 121(6):e26290:1–e26290:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVc

[Ano21r] Anonymous. Cover image, volume 121, issue 7. *International Journal of Quantum Chemistry*, 121(7):e26292:1–e26292:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVd

[Ano21s] Anonymous. Cover image, volume 121, issue 8. *International Journal of Quantum Chemistry*, 121(8):e26294:1–e26294:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:CIVe

[Ano21t] Anonymous. Cover image, volume 121, issue 9. *International Journal of Quantum Chemistry*, 121(9):e26296:1–e26296:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIa

[Ano21u] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(1):e26279:1–e26279:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIb

[Ano21v] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(2):e26281:1–e26281:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIc

[Ano21w] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(3):e26283:1–e26283:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IId

[Ano21x] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(4):e26285:1–e26285:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIe

[Ano21y] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(5):e26287:1–e26287:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIf

[Ano21z] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(6):e26289:1–e26289:??, March 15,

2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIg

[Ano21-27] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(7):e26291:1–e26291:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIh

[Ano21-28] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(8):e26293:1–e26293:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIi

[Ano21-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(9):e26295:1–e26295:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIj

[Ano21-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(10):e26297:1–e26297:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIk

[Ano21-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(11):e26299:1–e26299:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIl

[Ano21-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(12):e26301:1–e26301:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIm

[Ano21-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(13):e26303:1–e26303:??, July 5,

2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIn

[Ano21-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(14):e26305:1–e26305:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIo

[Ano21-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(15):e26307:1–e26307:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIp

[Ano21-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(16):e26309:1–e26309:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIq

[Ano21-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(17):e26311:1–e26311:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIr

[Ano21-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(18):e26313:1–e26313:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIs

[Ano21-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(19):e26315:1–e26315:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIt

[Ano21-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(20):e26317:1–e26317:??, October

15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIu

[Ano21-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(21):e26319:1–e26319:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIv

[Ano21-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(22):e26321:1–e26321:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIw

[Ano21-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(23):e26323:1–e26323:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2021:IIx

[Ano21-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 121(24):e26325:1–e26325:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:ESB

[Ano22a] Anonymous. Erratum: [Simon Brezovnik and Niko Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, IJQC **121**(6) 2021, e26530]. *International Journal of Quantum Chemistry*, 122(10):e26903:1–e26903:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BT21].

Anonymous:2022:IIa

[Ano22b] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(1):e26691:1–e26691:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIb

[Ano22c] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(2):e26693:1–e26693:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIc

[Ano22d] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(3):e26695:1–e26695:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IId

[Ano22e] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(4):e26697:1–e26697:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIe

[Ano22f] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(5):e26699:1–e26699:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIf

[Ano22g] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(6):e26701:1–e26701:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIg

[Ano22h] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(7):e26703:1–e26703:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIh

[Ano22i] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(8):e26705:1–e26705:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIi

[Ano22j] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(9):e26707:1–e26707:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIj

[Ano22k] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(10):e26709:1–e26709:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIk

[Ano22l] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(11):e26711:1–e26711:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIl

[Ano22m] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(12):e26713:1–e26713:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIm

[Ano22n] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(13):e26716:1–e26716:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2022:IIn

[Ano22o] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 122(14):e26717:1–e26717:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arrue:2020:RAA

[APR20] Lily Arrué and Ricardo Pino-Rios. Revisiting (anti)aromaticity and chemical bond in planar B_XN_X clusters ($x = 2$–11). *International Journal of Quantum Chemistry*, 120(22): e26403:1–e26403:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alvarado:2021:AAG

[ARBM21] Raúl Alvarado, Nicolás Ramos-Berdullas, and Marcos Mandado. On the adsorption affinity of graphene and white graphene sheets by dioxin-like pollutants. *International Journal of Quantum Chemistry*, 121(9):e26591:1–e26591:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ariyarathna:2021:SNM

[Ari21] Isuru R. Ariyarathna. Superatomic nature of metal encapsulated dodecahedrane: the case of $M@C_{20}H_{20}$ (M = Li, Na, Mg^{+}). *International Journal of Quantum Chemistry*, 121(20):e26774:1–e26774:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azzouz-Rached:2021:PDT

[ARRB+21] Ahmed Azzouz-Rached, Habib Rached, Majibul Haque Babu, Tariq Hadji, and Djamel Rached. Prediction of double transition metal $(Cr_{1-x}Zr_{x})_2$ AlC MAX phases as thermal barrier coatings: Insight from density functional theory. *International Journal of Quantum Chemistry*, 121(20):e26770:1–e26770:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alikhani:2022:ISB

[AS22] M. Esmail Alikhani and Bernard Silvi. Isomerism in secondary bonded complexes: Do structural rules apply? *International Journal of Quantum Chemistry*, 122(8):e26670:1–e26670:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albrecht-Schmitt:2020:TEC

[ASHPHCB20] Thomas E. Albrecht-Schmitt, David E. Hobart, Dayan Páez-Hernández, and Cristian Celis-Barros. Theoretical examination of covalency in berkelium (IV) carbonate complexes. *International Journal of Quantum Chemistry*, 120 (15):e26254:1–e26254:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andres:2022:BET

[ASO+22] Juan Andrés, Vicent S. Safont, Mónica Oliva, Kacee L. Caster, and Fabien Goulay. A bonding evolution theory study of the reaction between methylidyne radical, $CH(X^2\Pi)$, and cyclopentadiene, C_5H_6. *International Journal of Quantum Chemistry*, 122(11):e26892:1–e26892:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2020:IDC

[ATL+20] Diego R. Alcoba, Alicia Torre, Luis Lain, Ofelia B. Oña, Elías Ríos, and Gustavo E. Massaccesi. Incorporating dynamic correlation into the variational determination method of the second-order reduced density matrix in the doubly occupied configuration interaction space. *International Journal of Quantum Chemistry*, 120(15):e26256:1–e26256:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boda:2021:DFT

[BA21] Anil Boda and Sk. Musharaf Ali. Density functional theoretical tailoring of electronic effect through various substituents on calix[4]arene-crown-6 for efficient Cs^+ ion encapsulation and extraction. *International Journal of Quantum Chemistry*, 121(2):e26436:1–e26436:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barp:2022:EPE

[BA22a] Marcos V. Barp and Felipe Arretche. Electron and positron elastic scattering by non-central potentials: Matrix elements and symmetry properties in the first Born approximation. *International Journal of Quantum Chemistry*, 122 (13):e26909:1–e26909:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barp:2022:YTI

[BA22b] Marcos V. Barp and Felipe Arretche. Young-type interference in soft lepton scattering of diatomic homonuclear molecules. *International Journal of Quantum Chemistry*, 122(10):e26882:1–e26882:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bahar:2022:EOR

[Bah22] Mustafa Kemal Bahar. Erratum to: Optical response of plasma processed quantum dot under the external fields. *International Journal of Quantum Chemistry*, 122(9): e26893:1–e26893:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [KB21].

Ben-Asher:2020:CAP

[BAM20] Anael Ben-Asher and Nimrod Moiseyev. Complex absorbing potentials for Stark resonances. *International Journal of Quantum Chemistry*, 120(2):e26067:1–e26067:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouras:2020:ISM

[BB20] Farida Bouras and Ali Bentouaf. Investigation of structural and magnetoelectronic properties of new half-metallic Heusler alloys $Ru_2VGe_xSb_{1-x}$ ($x = 0$, 0.5 and 1): a density functional theory study. *International Journal of Quantum Chemistry*, 120(24):e26413:1–e26413:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benaissa:2021:TSM

[BBAA21] Abdelghani Benaïssa, Ali Bentouaf, Brahim Aïssa, and Boucif Abbar. Theoretical study of magneto-electronic properties of $TmCo_2$ and $NdCo_2$ intermetallic compounds through density functional theory calculations. *International Journal of Quantum Chemistry*, 121(5):e26488:1–e26488:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buzzanca:2020:ICE

[BBG20] Marissa Buzzanca, Brandon Brummeyer, and Jonathan H. Gutow. Improving convergence of experimental and computed vertical ionization energies using the ionization potential equation-of-motion coupled-cluster with singles and doubles method. *International Journal of Quantum Chemistry*, 120(18):e26261:1–e26261:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barysz:2021:AMR

[BCKN21] Maria Barysz, Ivan Cernusák, Vladimir Kellö, and Pavel Neogrády. AuSi molecule revisited: IOTC/CASSCF/CASPT2 calculations. *International Journal of Quantum Chemistry*, 121(5):e26502:1–e26502:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bako:2022:ICD

[BCM+22] Imre Bakó, Dániel Csókás, István Mayer, Szilvia Pothoczki, and László Pusztai. The influence of cations on the dipole moments of neighboring polar molecules. *International Journal of Quantum Chemistry*, 122(8):e26758:1–e26758:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balachandran:2021:EGG

[BDEM21] Selvaraj Balachandran, Hanyuan Deng, Suresh Elumalai, and Toufik Mansour. Extremal graphs on geometric-arithmetic index of tetracyclic chemical graphs. *International Journal of Quantum Chemistry*, 121(5):e26516:1–e26516:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Biag:2022:SLE

[BGK+22] Maryam Biag, Ammal Ghaffar, Muhammad Aslam Khan, Farooq Khan, and Shanawer Niaz. Slow light effect in hybrid optomechanical system. *International Journal of Quantum Chemistry*, 122(1):e26814:1–e26814:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ball:2020:EUS

[BHH20] K. Aurelia Ball, Kedan He, and Heidi P. Hendrickson. Engaging undergraduate students in computational chemistry research: a tutorial for new assistant professors. *International Journal of Quantum Chemistry*, 120(20):e26341:1–e26341:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bose:2021:QCP

[BM21] Amartya Bose and Nancy Makri. Quantum-classical path integral evaluation of reaction rates with a near-equilibrium flux formulation. *International Journal of Quantum Chemistry*, 121(10):qua26618:1–qua26618:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharyya:2020:NRP

[BMF20] Sukhamoy Bhattacharyya, Prasanta K. Mukherjee, and Burkhard Fricke. Nonlinear response properties of atomic hydrogen under quantum plasma environment: a time-dependent variation perturbation study on hyperpolarizability and two-photon excitations. *International Journal of Quantum Chemistry*, 120(24):e26422:1–e26422:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bones:2021:ECV

[BMH21] Don X. Bones, Justin T. Malme, and Erik P. Hoy. Examining conductance values in the biphenyl molecular switch with reduced density matrices. *International Journal of Quantum Chemistry*, 121(11):e26633:1–e26633:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bermudo:2021:OHC

[BMR21] Sergio Bermudo, Juan Monsalve, and Juan Rada. Orientations of hexagonal chains with extremal values of the Randić index. *International Journal of Quantum Chemistry*, 121(18):e26744:1–e26744:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bozkaya:2021:MFC

[Boz21] Ugur Bozkaya. Molint 1.0: a framework for the computation of molecular integrals and their derivatives for density-fitted methods. *International Journal of Quantum Chemistry*, 121 (11):e26623:1–e26623:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

BenSadok:2020:ECN

[BPB+20] Raouia Ben Sadok, Neculai Plugaru, Anca Birsan, Victor Kuncser, and Dalila Hammoutène. Effect of chemical nature of atoms on the electronic, dielectric, and dynamical properties of ABX_3 halide perovskite. *International Journal of Quantum Chemistry*, 120(10):e26172:1–e26172:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandan:2021:NIC

[Bra21] Silvia Antonia Brandán. Normal internal coordinates, force fields, and vibrational study of species derived from antiviral adamantadine. *International Journal of Quantum Chemistry*, 121(2):e26425:1–e26425:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boomadevi:2021:BRG

[BRB+21] Shanmugam Boomadevi, Mohanraj Ramachandran, Karuppannan Balamurugan, Dipali Nayak, Rajalingam Thangavel, Krishnamoorthy Pandiyan, Sambandam Anandan, and Dilibabu Sastikumar. Book review: *Growth, crystal structure, thermal, spectral studies and density functional theory computational analysis of an organic nonlinear optical crystal: 2-3-[2-(4-dimethylaminophenyl)vinyl]-5,5-dimethylcyclohex-2-enylidene-malonitrile*. *International Journal of Quantum Chemistry*, 121(17):e26741:1–e26741:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buchel:2021:DQM

[BRF21] Ralf C. Büchel, Dominik A. Rudolph, and Irmgard Frank. Deterministic quantum mechanics: the role of the Maxwell–Boltzmann distribution. *International Journal of Quantum Chemistry*, 121(7):e26555:1–e26555:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bautista-Renedo:2022:DCT

[BRHECY+22] Joanatan-Michael Bautista-Renedo, Raymundo Hernández-Esparza, Erick Cuevas-Yañez, Horacio Reyes-Pérez, Rubicelia Vargas, Jorge Garza, and Nelly González-Rivas. Deformations of cyclodextrins and their influence to form inclusion compounds. *International Journal of Quantum Chemistry*, 122(6):e26859:1–e26859:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bazargan:2020:IRP

[BS20] Gloria Bazargan and Karl Sohlberg. Influence of ring position on the temporal dependence of charge movement in a switchable [2]rotaxane. *International Journal of Quantum Chemistry*, 120(2):e26078:1–e26078:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buczek:2021:IFC

[BSH+21] Aneta Buczek, Monika Sta's, Christian Hebenstreit, Corina Maller, Małgorzata A. Broda, Teobald Kupka, and Anne-Marie Kelterer. Interaction of 5-fluorouracil with β-cyclodextrin: a density functional theory study with dispersion correction. *International Journal of Quantum Chemistry*, 121(5):e26487:1–e26487:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2021:EAS

[BSS21] Labanya Bhattacharya, Sagar Sharma, and Sridhar Sahu. Enhancement of air stability and photovoltaic performance in organic solar cells by structural modulation of bis-amide-based donor-acceptor copolymers: a computational insight. *International Journal of Quantum Chemistry*, 121 (6):e26524:1–e26524:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brezovnik:2021:GCM

[BT21] Simon Brezovnik and Niko Tratnik. General cut method for computing Szeged-like topological indices with applications to molecular graphs. *International Journal of Quantum Chemistry*, 121(6):e26530:1–e26530:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum about errors in mathematical expressions [Ano22a].

Butera:2021:MIE

[BTS+21] Valeria Butera, Yusuke Tanabe, Yu Shinke, Tomohisa Miyazawa, Tadahiro Fujitani, Megumi Kayanuma, and

Yoong-Kee Choe. Mechanistic investigation on ethanol-to-butadiene conversion reaction over metal oxide clusters. *International Journal of Quantum Chemistry*, 121(5): e26494:1–e26494:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bahar:2020:MOS

[BU20] Mustafa Kemal Bahar and Fatih Ungan. Magneto-optical specifications of Rosen–Morse quantum dot with screw dislocation. *International Journal of Quantum Chemistry*, 120 (11):e26186:1–e26186:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Badanko:2022:TAC

[BUF+22] Péter Badankó, Otabek Umarov, Csaba Fábri, Gábor J. Halász, and Ágnes Vibók. Topological aspects of cavity-induced degeneracies in polyatomic molecules. *International Journal of Quantum Chemistry*, 122(8):e26750:1–e26750:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bahar:2021:OAQ

[BUKA21] M. K. Bahar, F. Ungan, H. Kaya, and S. Akkoyun. Optical analysis of quantum dot with velocity-dependent potential. *International Journal of Quantum Chemistry*, 121(5): e26518:1–e26518:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benda:2022:PIS

[BVL22] Robert Benda, Thomas Vezin, and Bérengère Lebental. Prediction of the interaction strength of an urea-based probe toward ions in water by means of Density Functional Theory/Polarizable Continuum Model calculations. *International Journal of Quantum Chemistry*, 122(12):e26901:1–e26901:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borislavov:2020:TDR

[BVT20] Lyuben Borislavov, Zhivko Velkov, and Alia Tadjer. Topology delimited radical-scavenging propensity of monohydroxycinnamic acids. *International Journal of Quantum Chemistry*, 120(22):e26329:1–e26329:??, November 15, 2020. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boydas:2021:IXR

[BWBR21] Esma Birsen Boydas, Bernd Winter, David Batchelor, and Michael Roemelt. Insight into the X-ray absorption spectra of Cu-porphyrazines from electronic structure theory. *International Journal of Quantum Chemistry*, 121(3):e26515:1–e26515:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2022:SDI

[BWLZ22] Huiting Bian, Yongjin Wang, Jing Li, and Jun Zhao. Structure-dependence in initial decomposition of trans-1,2-dimethylcyclohexyl isomers: Kinetic exploration and conformational analysis. *International Journal of Quantum Chemistry*, 122(11):e26890:1–e26890:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bacalis:2022:VFE

[BXWK22] Naoum C. Bacalis, Zhuang Xiong, Zhen Xin Wang, and Dimitris Karaoulanis. Variational functionals for excited state saddle points versus traditional Hylleraas–Undheim and McDonald higher "roots," and a way to instantly improve a lowest state crude approximant. *International Journal of Quantum Chemistry*, 122(6):e26855:1–e26855:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2020:IRM

[BZP+20] He Bian, Honghong Zhang, Ling Pei, Qian Wang, Fang Wang, Yun Zhang, and Jinshe Chen. Insight into the reaction mechanism of CH_2SH with HO_2: a density functional theory study. *International Journal of Quantum Chemistry*, 120(8):e26146:1–e26146:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bai:2020:ICE

[BZW+20] Rui-Rong Bai, Cai-Rong Zhang, You-Zhi Wu, Li-Hua Yuan, Mei-Ling Zhang, Yu-Hong Chen, Zi-Jiang Liu, and Hong-Shan Chen. Interface configuration effects on excitation, exciton dissociation, and charge recombination in organic photovoltaic heterojunction. *International Journal of Quantum*

Chemistry, 120(4):e26103:1–e26103:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2021:CSI

[BZW+21] Huiting Bian, Yifan Zhang, Yongjin Wang, Jun Zhao, Xiaohui Ruan, and Jing Li. Computational study of inversion-topomerization pathways in 1,3-dimethylcyclohexane and 1,4-dimethylcyclohexane: Ab initio conformational analysis. *International Journal of Quantum Chemistry*, 121(11): e26636:1–e26636:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Choluj:2021:PII

[CBB21] Marta Chołuj, Bartosz Błasiak, and Wojciech Bartkowiak. Partitioning of the interaction-induced polarizability of molecules in helium environments. *International Journal of Quantum Chemistry*, 121(6):e26544:1–e26544:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Couty:2020:TIB

[CBK+20] François Couty, Oleg N. Burov, Mikhail E. Kletskii, Anton V. Lisovin, Karen Wright, Bruno Drouillat, and Sergey V. Kurbatov. Theoretical investigation of von Braun and von Braun-like reactions. *International Journal of Quantum Chemistry*, 120(3):e26088:1–e26088:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2020:IDF

[CCZ20] Wenlan Chen, Zhiqian Chen, and Shaohui Zheng. The influence of driving force on intramolecular electron transfer: a theoretical study of subphthalocyanine-AzaBODIPY-C_{60} supramolecular triad. *International Journal of Quantum Chemistry*, 120(7):e26131:1–e26131:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:CDS

[CDG+21] Jitian Chen, Tianyu Du, Liuzhou Gao, Zhongjing Chai, and Hao Dong. Computation-driven synthesis of pentothal sodium. *International Journal of Quantum Chemistry*, 121

(11):e26624:1–e26624:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz:2020:LBN

[CDR20] Roberto Cruz, Frank Duque, and Juan Rada. Lower bounds for the number of inlets of hexagonal systems. *International Journal of Quantum Chemistry*, 120(19):e26358:1–e26358:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carrier:2020:BAE

[CFJ20] Laurie Carrier, Charles-Émile Fecteau, and Paul A. Johnson. Bethe ansatz of electrons as a mean-field wavefunction for chemical systems. *International Journal of Quantum Chemistry*, 120(15):e26255:1–e26255:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chamorro:2021:MHH

[CFM+21] Yuly Chamorro, Edison Flórez, Alejandro Maldonado, Gustavo Aucar, and Albeiro Restrepo. Microsolvation of heavy halides. *International Journal of Quantum Chemistry*, 121 (7):e26571:1–e26571:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chamkin:2021:BDC

[Cha21a] Aleksandr A. Chamkin. Benchmarking DFT calculations of ^{1}H and ^{13}C chemical shifts in monosubstituted ferrocenes. *International Journal of Quantum Chemistry*, 121(4):e26456:1–e26456:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chan:2021:ADD

[Cha21b] Bun Chan. Assessment and development of DFT with the expanded CUAGAU-2 set of group-11 cluster systems. *International Journal of Quantum Chemistry*, 121(4): e26453:1–e26453:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cinal:2020:CDI

[Cin20] Marek Cinal. Comment on “Depurated inversion method for orbital-specific exchange potentials”. *International Journal* of *Quantum Chemistry*, 120(4):e26101:1–e26101:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See reply [MMM20].

Cioslowski:2022:REQ

[Cio22] Jerzy Cioslowski. Reverse engineering in quantum chemistry: How to reveal the fifth-order off-diagonal cusp in the one-electron reduced density matrix without actually calculating it. *International Journal of Quantum Chemistry*, 122 (8):e26651:1–e26651:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:RMB

[CL21] Yu Chen and Yunhua Liao. Rank of a matrix of block graphs. *International Journal of Quantum Chemistry*, 121 (18):e26748:1–e26748:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:IEZ

[CLC$^+$21] Zhicheng Chen, Yuhang Li, Yonghai Cao, Qiao Zhang, Hao Yu, and Feng Peng. Inhibitory effect of Zn^{2+} on the chain-initiation process of cumene oxidation. *International Journal of Quantum Chemistry*, 121(21):e26780:1–e26780:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chi:2020:CTB

[CLL20] Zongqing Chi, Qingzhong Li, and Hai-Bei Li. Comparison of triel bonds with different chalcogen electron donors: Its dependence on triel donor and methyl substitution. *International Journal of Quantum Chemistry*, 120(1):e26046:1–e26046:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cui:2021:EVD

[CLLC21] Xing-Hao Cui, Xiao-Hong Li, Shan-Shan Li, and Hong-Ling Cui. The effect of vacancy defect on quantum capacitance, electronic and magnetic properties of Sc_2CF_2 monolayer. *International Journal of Quantum Chemistry*, 121 (14):e26666:1–e26666:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2022:DVM

[CLS+22] Zhan-Bin Chen, Peng-Fei Liu, Hua-Yang Sun, Yue-Ying Qi, Guo-Peng Zhao, Xiao-Zhi Shen, Li-Guang Jiao, Kun Ma, Kai Wang, and Xiang-Dong Li. Development of various methods to the investigation of the spectral properties and collision dynamics of H-like ions taking place in dense and hot plasma environments. *International Journal of Quantum Chemistry*, 122(4):e26842:1–e26842:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chatterjee:2021:DAR

[CLW21] Subhojyoti Chatterjee, Fengyi Liu, and Feng Wang. Differentiation of alkyl radicals: a route through chemical graph theory. *International Journal of Quantum Chemistry*, 121 (7):e26567:1–e26567:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cherkaoui:2021:CRU

[CM21] Mustapha Cherkaoui and El Hassane Mourid. Correcting the representations used in teaching fundamentals of quantum spin to undergraduate and graduate students. *International Journal of Quantum Chemistry*, 121(19):e26755:1–e26755:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cherchab:2021:RSE

[CMGH+21] Youcef Cherchab, Ali Mir, Rafael González-Hernández, Khedija Talbi, and Abderrahim Bennadji. The role of the Scandium element concentration in the YN matrix: Ab initio study of structural, electronic, mechanical and thermal properties. *International Journal of Quantum Chemistry*, 121(22):e26791:1–e26791:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2021:NAD

[CMM21] Pedro J. Castro, Satoshi Maeda, and Keiji Morokuma. Nonadiabatic dynamic of atmospheric unimolecular photochemical reactions of 4,4-difluoro-crotonaldehyde using TD-DFT and TSH approaches. *International Journal of Quantum Chemistry*, 121(14):e26663:1–e26663:??, July 15, 2021. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cuesta:2022:USR

[CMM+22] Sebastián A. Cuesta, José R. Mora, Lorena M. Meneses, Edgar A. Márquez, Virginia Flores-Morales, Luis Rincón, Fernando J. Torres, and Cesar H. Zambrano. Unveiling the structure-reactivity relationship involved in the reaction mechanism of the HCl-catalyzed alkyl *t*-butyl ethers thermal decomposition. A computational study. *International Journal of Quantum Chemistry*, 122(14):e26915:1–e26915:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castanedo:2022:RPC

[CMY22] Lázaro A. M. Castanedo, Chérif F. Matta, and Kai E. O. Ylijoki. The reaction path of cyclooctatetraene dimerization revisited. *International Journal of Quantum Chemistry*, 122 (7):e26866:1–e26866:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas:2021:ACC

[CN21] Gustavo Cárdenas and Juan J. Nogueira. An algorithm to correct for the CASSCF active space in multiscale QM/MM calculations based on geometry ensembles. *International Journal of Quantum Chemistry*, 121(6):e26533:1–e26533:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cooper:2022:IIM

[CPK22] David L. Cooper, Robert Ponec, and Peter B. Karadakov. Investigating István Mayer's "improved" definitions of bond orders and free valence for correlated singlet-state wave functions. *International Journal of Quantum Chemistry*, 122(8): e26612:1–e26612:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chettri:2021:IMS

[CPL+21] B. Chettri, Prof. P. K. Patra, Lalmuanchhana, Lalhriatzuala, Swati Verma, B. Keshav Rao, Mohan L. Verma, Vishal Thakur, Narender Kumar, Nguyen N. Hieu, and D. P. Rai. Induced magnetic states upon electron-hole injection at B and N sites of hexagonal boron nitride bilayer: a density functional theory study. *International Journal of Quantum Chemistry*, 121(16):e26680:1–e26680:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calixto:2021:ABT

[CRC21] Manuel Calixto, Elvira Romera, and Octavio Castaños. Analogies between the topological insulator phase of 2D Dirac materials and the superradiant phase of atom-field systems. *International Journal of Quantum Chemistry*, 121(4):e26464:1–e26464:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carey:2021:VNS

[CRKMC21] Desmond MacLeod Carey, Peter L. Rodríguez-Kessler, and Alvaro Muñoz-Castro. Visualizing NMR-shielding effect in fullerene-ZnPc aggregates: Characteristic patterns of ZnP-based hosts and encapsulation nature from DFT calculations. *International Journal of Quantum Chemistry*, 121 (5):e26500:1–e26500:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz:2021:EVV

[CSGR21] Roberto Cruz, Andrés David Santamaría-Galvis, and Juan Rada. Extremal values of vertex-degree-based topological indices of coronoid systems. *International Journal of Quantum Chemistry*, 121(6):e26536:1–e26536:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheranovskii:2021:QPT

[CSK21] Vladyslav O. Cheranovskii, Viktor V. Slavin, and Douglas J. Klein. Quantum-phase transitions in 1D Heisenberg spin systems. *International Journal of Quantum Chemistry*, 121 (5):e26498:1–e26498:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:VAP

[CSS$^+$21] Chang-Yuan Chen, Dong-Sheng Sun, Guo-Hua Sun, Xiao-Hua Wang, Yuan You, and Shi-Hai Dong. The visualization of the angular probability distribution for the angular Teukolsky equation with $m \neq 0$. *International Journal of Quantum Chemistry*, 121(6):e26546:1–e26546:??, March 15,

2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chu:2021:EPH

[CSY+21] Yun-Jie Chu, Gang Sun, Chun-Hua Yang, Xue-Mei Chen, and Chun-Guang Liu. Epoxidation of propylene by hydrogen peroxide catalyzed by the silanol-functionalized polyoxometalates-supported ferrate: Electronic structure, bonding feature, and reaction mechanism. *International Journal of Quantum Chemistry*, 121(4):e26463:1–e26463:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2020:ESR

[CWY+20] Chang-Yuan Chen, Xiao-Hua Wang, Yuan You, Guo-Hua Sun, and Shi-Hai Dong. Exact solutions of the rigid rotor in the electric field. *International Journal of Quantum Chemistry*, 120(18):e26336:1–e26336:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:DFT

[CXZ+21] Yang Chen, Donghui Xu, Shuang Zhang, Ruolan Tan, Laicai Li, and Xiang-Yang Liu. Density functional theory calculations on the adsorption and degradation characteristics of ronidazole on the TiO_2 surface. *International Journal of Quantum Chemistry*, 121(13):e26648:1–e26648:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2020:TSI

[CYJC20] Lei Chen, Hui-Qing Yang, Cheng-Yu Jin, and Zhao-Xu Chen. Theoretical studies on the influence of metallic cations on ring opening of propylene oxide catalyzed by metal-salen complexes. *International Journal of Quantum Chemistry*, 120(22):e26366:1–e26366:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2021:SIM

[CZ21] Xue Chen and Shaohui Zheng. On the study of influence of molecular arrangements and dipole moment on exciton binding energy in solid state. *International Journal of Quantum Chemistry*, 121(5):e26511:1–e26511:??, March 5, 2021.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chu:2021:IBS

[CZW21] Xiumei Chu, Wenjuan Zhu, and Wenji Wang. Influence of bridge-state energy on the electron transfer relaxation and dephasing rate in a donor-bridge-acceptor system. *International Journal of Quantum Chemistry*, 121(22):e26795:1–e26795:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2020:HSH

[dAOdASP+20] Alan Leone de Araujo Oliveira, Mônica de Abreu Silva, Fernando Pirani, Luiz Guilherme Machado de Macedo, and Ricardo Gargano. Hydrogen sulphide H_2S and noble gases (Ng = He, Ne, Ar, Kr, Xe, Rn) complexes: a theoretical study of their dynamics, spectroscopy, and interactions. *International Journal of Quantum Chemistry*, 120(16):e26266:1–e26266:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2021:FTE

[DAR+21] Zhibin Du, Akbar Ali, Rabbia Rafee, Zahid Raza, and Muhammad Kamran Jamil. On the first two extremum Zagreb indices and coindices of chemical trees. *International Journal of Quantum Chemistry*, 121(6):e26547:1–e26547:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daud:2021:CQW

[Dau21] Mohammad Noh Daud. Controlling quantum wave packet of electronic motion on field-dressed Coulomb potential of H_2^+ by carrier-envelope phase-dependent strong field laser pulses. *International Journal of Quantum Chemistry*, 121(21):e26783:1–e26783:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Didar:2020:MDC

[DB20] Behnaz Rahmani Didar and Perla B. Balbuena. Methane dehydrogenation on Cu and Ni surfaces with low and moderate oxygen coverage. *International Journal of Quantum Chemistry*, 120(2):e26065:1–e26065:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Davidson:2022:VPA

[DC22] Ernest R. Davidson and Aurora E. Clark. A viewpoint on population analyses. *International Journal of Quantum Chemistry*, 122(8):e26860:1–e26860:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2021:ELS

[DCY21] Xueyan Dong, Lin Cheng, and Jucai Yang. Europium-linked structures and electronic properties of nanosize semiconductor $EuSi_n^{0/-}$ ($n = 11$–18) clusters. *International Journal of Quantum Chemistry*, 121(4):e26457:1–e26457:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dar:2022:HCL

[DDSB22] Mohammad Ovais Dar, Gurudutt Dubey, Tejender Singh, and Prasad V. Bharatam. N-heterocyclic carbene ligated oximes: Exploring the electronic structure and properties. *International Journal of Quantum Chemistry*, 122(13): e26907:1–e26907:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dubinets:2020:UEF

[DFB20] Nikita O. Dubinets, Alexandra Y. Freidzon, and Alexander A. Bagaturyants. Use of effective fragment potentials for simulation of excited states in an inhomogeneous environment. *International Journal of Quantum Chemistry*, 120(2): e26071:1–e26071:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diniakhmetova:2020:RFC

[DFK20] Diana R. Diniakhmetova, Anna K. Friesen, and Sergey V. Kolesov. Reactions of fullerene C_{60} with methyl methacrylate radicals: a density functional theory study. *International Journal of Quantum Chemistry*, 120(18):e26335:1–e26335:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2021:SHA

[DG21] Biswajit Das and Arijit Ghoshal. Stability of the helium atom embedded in classical nonideal plasmas. *Interna-*

tional Journal of Quantum Chemistry, 121(13):e26649:1–e26649:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2021:EAP

[DJC21] Jijun Ding, Yanxin Jin, and Haixia Chen. Electronic and adsorption properties of the zigzag-edged triangle graphene nanosheets. *International Journal of Quantum Chemistry*, 121(10):e26607:1–e26607:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dononelli:2021:ALB

[DK21] Wilke Dononelli and Thorsten Klüner. Analyzing the local basis set superposition error for CO adsorbed on rutile(110). *International Journal of Quantum Chemistry*, 121(2):e26428:1–e26428:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daengngern:2020:NQH

[DKK+20] Rathawat Daengngern, Osamu Kobayashi, Nawee Kungwan, Chanisorn Ngaojampa, and Masanori Tachikawa. Nuclear quantum and H/D isotope effects on three-centered bonding diborane: Path integral molecular dynamics simulations. *International Journal of Quantum Chemistry*, 120 (10):e26179:1–e26179:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2021:EMI

[DL21] Kecai Deng and Shuchao Li. Extremal Mostar indices of tree-like polyphenyls. *International Journal of Quantum Chemistry*, 121(9):e26602:1–e26602:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deLima:2020:CMR

[dLRdLJ+20] Filipe Belarmino de Lima, Gessenildo Pereira Rodrigues, Juracy Regis de Lucena Júnior, Elizete Ventura, Rui Fausto, Igor Reva, and Silmar Andrade do Monte. A comparative multi-reference configuration interaction study of the low-lying states of two thione isomers of thiophenol. *International Journal of Quantum Chemistry*, 120(16):e26263:1–e26263:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2021:ATD

[DLZ+21] Shizhi Dong, Yanshuai Li, Bingshuai Zhu, Ruichuan Li, Wenlong Shang, Linghui Chen, Jinyu Zhang, Zhilong Zhao, and Lin Guo. Application of two-dimensional sandwich structure supported Pt single-atom catalysts in photocatalytic hydrogen evolution: a first-principles study. *International Journal of Quantum Chemistry*, 121(23):e26800:1–e26800:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dohn:2020:MEE

[Doh20] Asmus O. Dohn. Multiscale electrostatic embedding simulations for modeling structure and dynamics of molecules in solution: a tutorial review. *International Journal of Quantum Chemistry*, 120(21):e26343:1–e26343:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

So:2020:CEP

[dOSdASC+20] Yuri A. de Oliveira Só, Mônica de Abreu Silva, Fernando M. Carvalho, Alessandra S. Kiametis, and Ricardo Gargano. Combining electronic properties and virtual screening for the development of new antioxidants: Trolox-like compounds as application example. *International Journal of Quantum Chemistry*, 120(11):e26194:1–e26194:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Devi:2020:DFT

[DPC+20] Assa Aravindh Sasikala Devi, Sakari Pallaspuro, Wei Cao, Mahesh Somani, Matti Alatalo, Marko Huttula, and Jukka Kömi. Density functional theory study of ω phase in steel with varied alloying elements. *International Journal of Quantum Chemistry*, 120(13):e26223:1–e26223:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zoua:2022:ABF

[dPZFM+22] Vincent de Paul Zoua, Aymard Didier Tamafo Fouegue, Désiré Bikélé Mama, Julius Numbonui Ghogomu, and Rahman Abdoul Ntieche. Ability of $B_{12}N_{12}$ fullerene like nanocage for sensing and improving the antioxidant activity of juglone and its derivative: Density functional theory investigation. *International Journal of Quantum Chemistry*, 122(4): e26843:1–e26843:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2021:FIN

[DQS+21] Sheng Ding, Muhammad Imran Qureshi, Syed Fehmeed Shah, Asfand Fahad, Muhammad Kamran Jamil, and Jia-Bao Liu. Face index of nanotubes and regular hexagonal lattices. *International Journal of Quantum Chemistry*, 121(19):e26761:1–e26761:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Neto:2021:TTD

[dRNS21] Armando S. de Rezende Neto and Leandro Seixas. Toward a two-dimensional NbS_2-based electrode for lithium-ion batteries. *International Journal of Quantum Chemistry*, 121(9): e26603:1–e26603:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Darvishnejad:2020:DFT

[DRV20] Mohammad Hossein Darvishnejad and Adel Reisi-Vanani. Density functional theory study of CO_2 capture and storage promotion using manipulation of graphyne by $3d$ and $4d$ transition metals. *International Journal of Quantum Chemistry*, 120(18):e26342:1–e26342:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dressler:2020:RER

[DS20] Christian Dreßler and Daniel Sebastiani. Reduced eigensystem representation of the linear density-density response function. *International Journal of Quantum Chemistry*, 120(3):e26085:1–e26085:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filho:2020:MCI

[dSFdSdMdM20] Antônio João da Silva Filho, Otávio Luís de Santana, Elizete Ventura do Monte, and Silmar Andrade do Monte. A multireference configuration interaction study with singles and doubles of some mesoionic rings: reaction and activation free energies for the ring-opening reaction. *Inter-*

national Journal of Quantum Chemistry, 120(23):e26391:1–e26391:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dreyse:2020:EDS

[DSNZ+20] Paulina Dreyse, Mireya Santander-Nelli, David Zambrano, Luis Rosales, and Luis Sanhueza. Electron-donor substituents on the dppz-based ligands to control luminescence from dark to bright emissive state in Ir(III) complexes. *International Journal of Quantum Chemistry*, 120 (12):e26167:1–e26167:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dedecek:2021:SDD

[DTAS21] Jiri Dedecek, Edyta Tabor, Prokopis C. Andrikopoulos, and Stepan Sklenak. Splitting dioxygen over distant binuclear transition metal cationic sites in zeolites. Effect of the transition metal cation. *International Journal of Quantum Chemistry*, 121(10):e26611:1–e26611:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2021:MTE

[DTW21] Hanyuan Deng, Zikai Tang, and Renfang Wu. Molecular trees with extremal values of Sombor indices. *International Journal of Quantum Chemistry*, 121(11):e26622:1–e26622:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2021:TEG

[DYG21] Xueyan Dong, Jucai Yang, and Mazhar Amjad Gilani. Theoretical exploration of global minima, magnetism, structural stability and growth pattern of holmium-doped silicon $HoSi_n^{0/-}$ ($n = 10$–18) nanoclusters. *International Journal of Quantum Chemistry*, 121(21):e26776:1–e26776:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diniakhmetova:2022:RSR

[DYK22] Diana R. Diniakhmetova, Rosa Kh. Yumagulova, and Sergey V. Kolesov. Reactivity of short radicals at the initial stages of radical polymerization of allyl chloride: Chain growth versus addition to fullerene. *International Journal of Quantum Chemistry*, 122(5):e26852:1–e26852:??, March 05,

2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estanon:2020:TDC

[EAPCD20] Carlos R. Estañón, Norberto Aquino, David Puertas-Centeno, and Jesus S. Dehesa. Two-dimensional confined hydrogen: an entropy and complexity approach. *International Journal of Quantum Chemistry*, 120(11):e26192:1–e26192:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estanon:2021:CRC

[EAPCD21] Carlos R. Estañón, Norberto Aquino, David Puertas-Centeno, and Jesus S. Dehesa. Crámer–Rao complexity of the confined two-dimensional hydrogen. *International Journal of Quantum Chemistry*, 121(2):e26424:1–e26424:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elder:2022:ALR

[EB22] Jesse B. Elder and Eric A. C. Bushnell. An assessment of long-range corrected density functional approximations in the calculation of the reduction potentials of $Ni(S_2C_2H_2)_2$, $Ni(Se_2C_2H_2)_2$, $Ni(S_2C_2H_2)(N_2C_2H_4)$, and $Ni(Se_2C_2H_2)(N_2C_2H_4)$ complexes. *International Journal of Quantum Chemistry*, 122(9):e26874:1–e26874:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ehn:2021:AIP

[ÉC21] Ladislav Éhn and Ivan Cernusák. Atomic and ionic polarizabilities of B, C, N, O, and F. *International Journal of Quantum Chemistry*, 121(4):e26467:1–e26467:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

ElHachimi:2021:EEP

[EGLJQ+21] Abdel Ghafour El Hachimi, Alfredo Guillén-López, Oscar A. Jaramillo-Quintero, Marina E. Rincón, Perla Yazmín Sevilla-Camacho, and Jesús Muñiz. Exploring the enhanced performance of Sb_2S_3/doped-carbon composites as potential anode materials for sodium-ion batteries: a density functional theory approach. *International Journal of Quantum*

Chemistry, 121(21):e26779:1–e26779:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ehlert:2020:ACS

[ELH20] Christopher Ehlert, Xiaojing J. Liu, and Ian P. Hamilton. Au_{21} cage structures and their magic number trications. *International Journal of Quantum Chemistry*, 120 (11):e26191:1–e26191:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Enchev:2021:BRE

[EM21] Venelin Enchev and Nadezhda Markova. Book review: *Effect of external electric field on the tautomeric equilibrium and structure of* 2*-carbamido-1,3-indandione*. *International Journal of Quantum Chemistry*, 121(19):e26760:1–e26760:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Evans:2020:UWE

[EPMC20] Rebecca Evans, Madison Perchik, Caroline Magee, and Mauricio Cafiero. Undergraduate women empowering women in computational chemistry: Three perspectives. *International Journal of Quantum Chemistry*, 120(20): e26354:1–e26354:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2022:COM

[ER22] Mehdi D. Esrafili and Farzad Arjomandi Rad. CO oxidation mediated by Al-doped ZnO nanoclusters: a first-principles investigation. *International Journal of Quantum Chemistry*, 122(9):e26873:1–e26873:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Enchev:2021:SCM

[ES21] Venelin Enchev and Sofia Slavova. Self-catalytic mechanism of prebiotic reactions: II. From urea and glycinamide to hypoxanthine. *International Journal of Quantum Chemistry*, 121(5):e26508:1–e26508:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Etienne:2020:CSC

[Eti20] Thibaud Etienne. A comprehensive, self-contained derivation of the one-body density matrices from single-reference excited-state calculation methods using the equation-of-motion formalism. *International Journal of Quantum Chemistry*, 120(5):e26110:1–e26110:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Forgionny:2020:TDE

[FAJOF20] Angélica Forgionny, Nancy Y. Acelas, Carlos Jimenez-Orozco, and Elizabeth Flórez. Toward the design of efficient adsorbents for Hg^{2+} removal: Molecular and thermodynamic insights. *International Journal of Quantum Chemistry*, 120(15):e26258:1–e26258:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fu:2022:CLV

[FCL22] Jia Fu, Su Chen, and Xing Liu. Calculation of lattice vibrational and thermal properties of cadmium sulfide nanocrystal and growth preference of cadmium sulfide powder during microwave-hydrothermal process. *International Journal of Quantum Chemistry*, 122(2):e26828:1–e26828:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fadili:2021:IPP

[FFBH21] Driss Fadili, Zakaria Mohyi Eddine Fahim, Si Mohamed Bouzzine, and Mohamed Hamidi. Improved photovoltaic performance of phosphonic acid-based sensitized solar cells via an electron-withdrawing moiety: a density of functional theory study. *International Journal of Quantum Chemistry*, 121(2):e26431:1–e26431:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frank:2020:AWH

[FGMO20] Irmgard Frank, Stefanie Genuit, Florian Matz, and Hedda Oschinski. Ammonia, water, and hydrogen: Can nuclear motion be described classically? *International Journal of Quantum Chemistry*, 120(7):e26142:1–e26142:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Folmsbee:2021:ACE

[FH21] Dakota Folmsbee and Geoffrey Hutchison. Assessing conformer energies using electronic structure and machine learning methods. *International Journal of Quantum Chemistry*, 121(1):e26381:1–e26381:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2021:ASM

[Fin21] Kati Finzel. Analytical shell models for light atoms. *International Journal of Quantum Chemistry*, 121(3):e26212:1–e26212:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Farrokhpour:2020:TSD

[FK20] Hossein Farrokhpour and Samaneh Khoshkhou. Theoretical study of the desorption of neutral and ionic alkali metal atoms from the excited Li^+ $(H_2\ O)_{n=1--4}$ and Na^+ $(H_2O)_{n=1-4}$ cluster models: Electronic excitation charge transfer. *International Journal of Quantum Chemistry*, 120(4):e26104:1–e26104:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fatima:2022:FPS

[FMH+22] Afrinish Fatima, Abdul Majid, Sajjad Haider, Muhammad Saeed Akhtar, and Mohammad Alkhedher. First principles study of layered silicon carbide as anode in lithium ion battery. *International Journal of Quantum Chemistry*, 122 (11):e26895:1–e26895:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filho:2021:SSE

[FPdS21] Luciano F. Filho, Fernando N. N. Pansini, and Fábio A. L. de Souza. Size and shape effects on the stability, electronic structure, and Raman spectroscopy of $(SrO)_n$ nanoclusters. *International Journal of Quantum Chemistry*, 121 (12):e26642:1–e26642:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fatima:2022:EPT

[FSR+22] Rida Fatima, Rao Aqil Shehzad, Alvina Rasool, Muhammad Yaseen, Saleem Iqbal, Muhammad Jawwad Saif, and Javed Iqbal. Exploring the potential of tetraazaacene derivatives as photovoltaic materials with enhanced photovoltaic parameters. *International Journal of Quantum Chemistry*, 122 (1):e26817:1–e26817:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fang:2021:EVS

[FYL21] Xiaona Fang, Lihua You, and Hechao Liu. The expected values of Sombor indices in random hexagonal chains, phenylene chains and Sombor indices of some chemical graphs. *International Journal of Quantum Chemistry*, 121(17):e26740:1–e26740:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2020:MDN

[FZL+20] Wen-Jie Fan, Dan Zhao, Na Liu, Da-Zhi Tan, and Yong-Gang Chen. Molecular design of novel indacenodithiophene-based organic dyes for efficient dye-sensitized solar cells applications. *International Journal of Quantum Chemistry*, 120(8):e26147:1–e26147:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grabarek:2020:IOT

[GA20] Dawid Grabarek and Tadeusz Andruniów. Illuminating the origins of two-photon absorption properties in fluorescent protein chromophores. *International Journal of Quantum Chemistry*, 120(3):e26086:1–e26086:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gall:2021:QCS

[GB21] Marian Gall and Martin Breza. Quantum-chemical study of octafluoro-spirobi[triphosphazene]. *International Journal of Quantum Chemistry*, 121(10):e26613:1–e26613:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Greene-Diniz:2021:GUC

[GDR21] Gabriel Greene-Diniz and David Muñoz Ramo. Generalized unitary coupled cluster excitations for multireference molecular states optimized by the variational quantum eigensolver. *International Journal of Quantum Chemistry*, 121(4):e26352:1–e26352:??, February 15, 2021. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghashghaee:2020:HIC

[GG20a] Mohammad Ghashghaee and Mehdi Ghambarian. Highly improved carbon dioxide sensitivity and selectivity of black phosphorene sensor by vacancy doping: a quantum chemical perspective. *International Journal of Quantum Chemistry*, 120(16):e26265:1–e26265:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gleeson:2020:TSE

[GG20b] Duangkamol Gleeson and Matthew Paul Gleeson. Theoretical studies to estimate the skin sensitization potential of chemicals of the Schiff base domain. *International Journal of Quantum Chemistry*, 120(12):e26218:1–e26218:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gulin-Gonzalez:2022:ACC

[GG22] Jorge Gulín-González. Achievement and challenges of the Cuban Science, Technology, and Innovation System: a perspective on computational science. *International Journal of Quantum Chemistry*, 122(3):e26837:1–e26837:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guler:2021:FPS

[GGUU21] Emre Güler, Melek Güler, Sule Ugur, and Gökay Ugur. First principles study of electronic, elastic, optical and magnetic properties of Rh_2MnX (X = Ti, Hf, Sc, Zr, Zn) Heusler alloys. *International Journal of Quantum Chemistry*, 121 (10):e26606:1–e26606:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Griego:2021:ACD

[GKK21] Charles D. Griego, John R. Kitchin, and John A. Keith. Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. *International Journal of Quantum Chemistry*, 121(1):e26380:1–e26380:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gallenkamp:2021:CCM

[GKPK21] Charlotte Gallenkamp, Ulrike I. Kramm, Jonny Proppe, and Vera Krewald. Calibration of computational Mössbauer spectroscopy to unravel active sites in FeNC catalysts for the oxygen reduction reaction. *International Journal of Quantum Chemistry*, 121(3):e26394:1–e26394:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2021:CCA

[GM21] I. I. Guseinov and B. A. Mamedov. Corrigendum to: "On the calculation of arbitrary multielectron molecular integrals over Slater-Type orbitals using recurrence relations for overlap integrals I. Single-Center expansion method" [Int. J. Quantum Chem., 78 (2000) 146–152]. *International Journal of Quantum Chemistry*, 121(13):e26640:1–e26640:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:2020:NCC

[GMO+20] Johanna Camacho Gonzalez, Sukanta Mondal, Fernanda Ocayo, Raul Guajardo-Maturana, and Alvaro Muñoz-Castro. Nature of C_{60} and C_{70} fullerene encapsulation in a porphyrin- and metalloporphyrin-based cage: Insights from dispersion-corrected density functional theory calculations. *International Journal of Quantum Chemistry*, 120(3): e26080:1–e26080:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guajardo-Maturana:2021:NCS

[GMRKMCMC21] Raul Guajardo-Maturana, Peter L. Rodríguez-Kessler, Desmond MacLeod-Carey, and Alvaro Muñoz-Castro. On the ^{13}C-NMR chemical shift anisotropy patterns and aromatic character in strained fullerenes: Computational analysis of D_{6h} /D_{2d}–C_{36} fullerene. *International Journal of Quantum Chemistry*, 121(2):e26437:1–e26437:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2020:ESS

[GN20] Piu Ghosh and Debraj Nath. Exact solutions and spectrum analysis of a noncentral potential in the presence of vector potential. *International Journal of Quantum Chemistry*, 120(9):e26153:1–e26153:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2021:GQS

[GN21a] Piu Ghosh and Debraj Nath. Generalized quantum similarity index: an application to pseudoharmonic oscillator with isospectral potentials in 3D. *International Journal of Quantum Chemistry*, 121(5):e26517:1–e26517:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2021:LER

[GN21b] Piu Ghosh and Debraj Nath. Localization effect on Rényi complexity of Kratzer potential in the presence of Aharonov–Bohm field. *International Journal of Quantum Chemistry*, 121(4):e26461:1–e26461:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghorai:2020:ISS

[GNC20] Sankar Ghorai, Pulak Naskar, and Pinaki Chaudhury. An investigation on the structure, spectroscopy, and thermodynamic aspects of $Cl_2^{(-1)}$ $(H_2O)_n$ clusters: a combined Parallel tempering and DFT based study. *International Journal of Quantum Chemistry*, 120(17):e26270:1–e26270:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goodwin:2020:SAC

[GOR20] Conrad A. P. Goodwin, Fabrizio Ortu, and Daniel Reta. Strangely attractive: Collaboration and feedback in the field of molecular magnetism. *International Journal of Quantum Chemistry*, 120(14):e26248:1–e26248:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gale:2020:CAW

[GOS20] Ariel G. Gale, Tuguldur T. Odbadrakh, and George C. Shields. Catalytic activity of water molecules in gas-phase glycine dimerization. *International Journal of Quantum Chemistry*, 120(20):e26469:1–e26469:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gotze:2021:UFP

[GPP+21] Jan P. Götze, Yuan-Wei Pi, Simon Petry, Fabian Langkabel, Jan Felix Witte, and Oliver Lemke. A user-friendly, Python-based quantum mechanics/Gromacs interface: gmx2qmmm. *International Journal of Quantum Chemistry*, 121(3):e26486:1–e26486:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez-Ramirez:2020:GPP

[GRFM20] Henry Nicole González-Ramírez and Roberto Flores-Moreno. A generalized any-particle propagator theory: Calculations of nucleon's binding energies. *International Journal of Quantum Chemistry*, 120(7):e26140:1–e26140:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2021:RGP

[GRLH21] Wei Gao, Lu-Lu Ren, Run-Qin Liu, and Yong-Chang Han. The role of geometric phase in dissociation dynamics of the D_2^+ molecule. *International Journal of Quantum Chemistry*, 121(22):e26787:1–e26787:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guan:2021:REP

[GRZ+21] Meihua Guan, Guangmin Ren, Xiaochao Zhang, Qirui Zhang, Changming Zhang, Rui Li, and Caimei Fan. Regulating electronic properties of BiOBr to enhance visible light response via 3d transition metals doping: DFT + U calculations. *International Journal of Quantum Chemistry*, 121(7):e26568:1–e26568:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2020:SRD

[GSMT+20] Victor García, Jesús Sánchez-Márquez, Estefanía Torres, David Zorrilla, and Manuel Fernández. Spatially restricted Double Z-Simplified Box Orbital basis sets: Optimization and comparison with some standard basis sets. *International Journal of Quantum Chemistry*, 120(6):e26129:1–e26129:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gourav:2022:FPI

[GSRG22] Gourav, Mukaddar Sk, Krishnamoorthy Ramachandran, and Saurabh Ghosh. First-principles investigation of $Rb_2Ag(Ga/In)Br_6$ for thermoelectric and photovoltaic applications. *International Journal of Quantum Chemistry*, 122(14):e26910:1–e26910:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grimmel:2020:IWG

[GTV20] Stephanie A. Grimmel, Tiago Q. Teodoro, and Lucas Visscher. Is it worthwhile to go beyond the local-density approximation in subsystem density functional theory? *International Journal of Quantum Chemistry*, 120(21):e26111:1–e26111:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gunko:2021:ACD

[Gun21] Vladimir M. Gun'ko. Atomic charge distribution functions as a tool to analyze electronic structure of molecular and cluster systems. *International Journal of Quantum Chemistry*, 121(14):e26665:1–e26665:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gan:2021:GSC

[GW21] Li-Hua Gan and Chun-Ru Wang. The generation, stability, and connectivity of small-sized carbon cages. *International Journal of Quantum Chemistry*, 121(4):e26462:1–e26462:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gong:2022:LSO

[GXL$^+$22] Lijing Gong, Jing Xu, Chunping Li, Xiangyu Zhang, and Zhi Jiang. Linear and second-order nonlinear optical properties of non-fullerene acceptor derivatives with A-D-A structure. *International Journal of Quantum Chemistry*, 122 (6):e26861:1–e26861:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gu:2020:SSE

[GYC20] Yansong Gu, Jucai Yang, and Lin Cheng. Structural stability and evolution of terbium-doped silicon clusters and influence of $4f \rightarrow 5d$ electronic transition mechanism on magnetism and appearance of photoelectron spectroscopy for $TbSi_n^{0/-}$ (n = 6–18) clusters. *International Journal of Quantum Chemistry*, 120(3):e26087:1–e26087:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2021:SBN

[GZC21] Peng Gao, Jie Zhang, and Hongming Chen. A systematic benchmarking of ^{31}P and ^{19}F NMR chemical shift predictions using different DFT/GIAO methods and applying linear regression to improve the prediction accuracy. *International Journal of Quantum Chemistry*, 121(5):e26482:1–e26482:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2022:CMO

[GZCY22] Meiqi Guo, Min Zhou, Shuo Chai, and Jie Yu. Controlling molecular orientation by laser pulses with two different envelope shapes. *International Journal of Quantum Chemistry*, 122(2):e26830:1–e26830:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2022:CSS

[GZWL22] Jingjing Guo, Huiyan Zhao, Jing Wang, and Ying Liu. Cu_nSi_{12} (n = 30, 38, and 60): a series of silicide cages with high content of TM atoms. *International Journal of Quantum Chemistry*, 122(13):e26905:1–e26905:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haoer:2021:WPS

[Hao21] Raad Sehen Haoer. Wiener polarity and similar topological descriptors of some product graphs. *International Journal of Quantum Chemistry*, 121(22):e26796:1–e26796:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Havare:2021:TIQ

[Hav21] Özge Çolakoğlu Havare. Topological indices and QSPR modeling of some novel drugs used in the cancer treatment. *International Journal of Quantum Chemistry*, 121 (24):e26813:1–e26813:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamli:2021:TIN

[HBB+21] Meryem Hamli, Djillali Bensaid, Amel Benkada, Nour eddine Bouzouira, Kadour Bencherif, and Fathi Benzoudji. Theoretical investigation of novel half Heusler compounds MRhSb (M = Nb and Ta): For optoelectronic and thermoelectric applications. *International Journal of Quantum Chemistry*, 121(13):e26656:1–e26656:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2020:IGM

[HBY20] Hong Huang, Xue Bai, and Lijun Yang. Intriguing generative metabolism discovery of reactive metabolite nitroso of lapatinib and relevant structural modification. *International Journal of Quantum Chemistry*, 120(12):e26210:1–e26210:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2020:IDR

[HCZ20] Yaosong Huang, Yugong Chen, and Mingfei Zhou. Identification of decomposition reactions for HMDSO organosilicon using quantum chemical calculations. *International Journal of Quantum Chemistry*, 120(24):e26415:1–e26415:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2021:EAN

[HDF+21] Na Hou, Fang-Yue Du, Ran Feng, Hai-Shun Wu, and Zhi-Ru Li. Effects of the atomic number of alkali atom and pore size of graphyne on the second-order nonlinear optical response of superalkali salts of graphynes OM_3^+ @GYs$^-$ (M = Li, Na, and K). *International Journal of Quantum Chemistry*, 121(4):e26477:1–e26477:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hanwell:2021:OCJ

[HHG+21] Marcus D. Hanwell, Chris Harris, Alessandro Genova, Mojtaba Haghighatlari, Muammar El Khatib, Patrick Avery, Johannes Hachmann, and Wibe Albert de Jong. Open Chemistry, JupyterLab, REST, and quantum chemistry. *International Journal of Quantum Chemistry*, 121

(1):e26472:1–e26472:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Horchani:2021:RVS

[HJIO21] Ridha Horchani, Haikel Jelassi, Akpan N. Ikot, and Uduakobong S. Okorie. Rotation vibration spectrum of potassium molecules via the improved generalized Pöschl–Teller oscillator. *International Journal of Quantum Chemistry*, 121 (7):e26558:1–e26558:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hegely:2022:MAI

[HK22] Bence Hégely and Mihály Kállay. Multilevel approach to the initial guess for self-consistent field calculations. *International Journal of Quantum Chemistry*, 122(8):e26782:1–e26782:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2020:DJT

[HL20] Zhishuo Huang and Dan Liu. Dynamical Jahn–Teller effect in the first excited C_{60}^{-}. *International Journal of Quantum Chemistry*, 120(8):e26148:1–e26148:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Han:2020:MSD

[HLL20a] Yanqiang Han, Jinyun Liu, and Jinjin Li. Molecular structure determination of solid carbon dioxide phase IV at high pressures and temperatures based on Møller–Plesset perturbation theory. *International Journal of Quantum Chemistry*, 120(23):e26397:1–e26397:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2020:HTB

[HLL20b] Mingchang Hou, Zhenbo Liu, and Qingzhong Li. The π-hole tetrel bond between X_2 TO and CO_2: Substituent effects and its potential adsorptivity for CO_2. *International Journal of Quantum Chemistry*, 120(15):e26251:1–e26251:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernandez-Martinez:2020:NDH

[HMBPJ+20] Laura Hernández-Martínez, Eric Brémond, Angel J. Pérez-Jiménez, Emilio San-Fabián, Carlo Adamo, and Juan C. Sancho-García. Nonempirical (double-hybrid) density functionals applied to atomic excitation energies: a systematic basis set investigation. *International Journal of Quantum Chemistry*, 120(11):e26193:1–e26193:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holtomo:2020:IPL

[HMN20] Olivier Holtomo, Ousmanou Motapon, and Mama Nsangou. Insight and performance of LC-DFT vs DFT in the NMR shielding and chemical shift calculations: Case of CHCl–CH–CF3. *International Journal of Quantum Chemistry*, 120(24):e26408:1–e26408:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoat:2021:FRS

[HNO+21] D. M. Hoat, Duy Khanh Nguyen, Vo Van On, Bakhtiar Ul Haq, J. F. Rivas-Silva, and Gregorio H. Cocoletzi. Feature-rich structural, electronic, magnetic and optical properties of the fluorine- and nitrogen-incorporated CaF_2 compound. *International Journal of Quantum Chemistry*, 121 (15):e26672:1–e26672:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hofener:2021:KPW

[Höf21] Sebastian Höfener. The KOALA program: Wavefunction frozen-density embedding. *International Journal of Quantum Chemistry*, 121(3):e26351:1–e26351:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Holloczki:2021:EPM

[Hol21] Oldamur Hollóczki. Evidence for protein misfolding in the presence of nanoplastics. *International Journal of Quantum Chemistry*, 121(3):e26372:1–e26372:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halbert:2020:CIV

[HOVG20a] Loïc Halbert, Małgorzata Olejniczak, Valérie Vallet, and André Severo Pereira Gomes. Cover image, volume 120, issue 21. *International Journal of Quantum Chemistry*, 120(21):e26496:1–e26496:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halbert:2020:ISE

[HOVG20b] Loïc Halbert, Małgorzata Olejniczak, Valérie Vallet, and André Severo Pereira Gomes. Investigating solvent effects on the magnetic properties of molybdate ions (MoO_4^{2-}) with relativistic embedding. *International Journal of Quantum Chemistry*, 120(21):e26207:1–e26207:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Helmich-Paris:2021:SXR

[HP21] Benjamin Helmich-Paris. Simulating X-ray absorption spectra with complete active space self-consistent field linear response methods. *International Journal of Quantum Chemistry*, 121(3):e26559:1–e26559:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Honore:2022:ENP

[HRA+22] Eduardo M. Honoré, Elías Ríos, Diego R. Alcoba, Gustavo E. Massaccesi, Alicia Torre, Luis Lain, and Ofelia B. Oña. Exploiting the nearsightedness principle within the framework of the anti-Hermitian contracted Schrödinger equation. *International Journal of Quantum Chemistry*, 122 (6):e26862:1–e26862:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hidalgo-Rosa:2020:SME

[HRTSS+20] Yoan Hidalgo-Rosa, Manuel A. Treto-Suárez, Eduardo Schott, Ximena Zarate, and Dayán Páez-Hernández. Sensing mechanism elucidation of a chemosensor based on a metal-organic framework selective to explosive aromatic compounds. *International Journal of Quantum Chemistry*, 120(23):e26404:1–e26404:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halasz:2022:LST

[HSV22] Gábor J. Halász, Tamás Szidarovszky, and Ágnes Vibók. On the line shape of the total rovibronic absorption in laser-dressed diatomic molecules. *International Journal of Quantum Chemistry*, 122(7):e26868:1–e26868:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haldar:2021:MFD

[HTNP21] Soumi Haldar, Kaushik Talukdar, Malaya K. Nayak, and Sourav Pal. Molecular frame dipole moment of diatomic molecules within relativistic coupled-cluster framework: a comparative study of expectation value versus energy derivative approach. *International Journal of Quantum Chemistry*, 121(20):e26764:1–e26764:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2020:WDB

[Hua20] Chen Huang. Wavelength-decomposition-based embedded cluster density approximation for systems with nonlocal electron correlation. *International Journal of Quantum Chemistry*, 120(21):e26347:1–e26347:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2021:PHE

[HW21a] Hua Hou and Baoshan Wang. Prediction on the high-energy density covalent organic frameworks with diamond network. *International Journal of Quantum Chemistry*, 121(22):e26790:1–e26790:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2021:SDM

[HW21b] Hua Hou and Baoshan Wang. Solvent-dependent mechanistic aspects for the redox reaction of paraquat in basic solution. *International Journal of Quantum Chemistry*, 121(19): e26757:1–e26757:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2021:FEM

[HYC+21] Wenhao Hu, Rourou Yu, Zhenxiang Chang, Zhaoyang Tan, and Xiuwu Liu. The fire extinguishing mechanism of ultrafine composite dry powder agent containing $Mg(OH)_2$. *International Journal of Quantum Chemistry*, 121(24):e26810:1–e26810:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2022:SDD

[HYHW22] Xiaoyi Hu, Xiaojuan Yu, Hua Hou, and Baoshan Wang. Stereo-dependent dimerization, boiling points, diffusion coefficients, and dielectric constants of E/Z-HFO-1234ze. *International Journal of Quantum Chemistry*, 122(5): e26848:1–e26848:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2020:TOL

[HYY20] Qiaoli Hu, Jiena Yun, and Gang Yang. Toward the origin of life over feldspar surfaces: Adsorption of amino acids and catalysis of conformational interconversions. *International Journal of Quantum Chemistry*, 120(10):e26175:1–e26175:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2021:BFS

[HZC21] Xia Huang, Hong Zhang, and Xin-Lu Cheng. Bandgaps in free-standing monolayer TiO_2: Ab initio diffusion quantum Monte Carlo study. *International Journal of Quantum Chemistry*, 121(12):e26643:1–e26643:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imran:2020:EMI

[IAI20] Muhammad Imran, Shehnaz Akhter, and Zahid Iqbal. Edge Mostar index of chemical structures and nanostructures using graph operations. *International Journal of Quantum Chemistry*, 120(15):e26259:1–e26259:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iribarne:2021:AOM

[ID21] Federico Iribarne and Pablo A. Denis. Adsorption of organic molecules on graphene and fluorographene: an unresolved discrepancy between experiment and theory. *International Journal of Quantum Chemistry*, 121(10):e26605:1–e26605:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imran:2021:STI

[IMJ21a] Muhammad Imran, Mehar Ali Malik, and Ramsha Javed. On Szeged-type indices of titanium oxide TiO_2 nanotubes. *International Journal of Quantum Chemistry*, 121(15): e26669:1–e26669:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imran:2021:WPI

[IMJ21b] Muhammad Imran, Mehar Ali Malik, and Ramsha Javed. Wiener polarity index and related molecular topological descriptors of titanium oxide nanotubes. *International Journal of Quantum Chemistry*, 121(11):e26627:1–e26627:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isukapalli:2022:CIV

[INV22a] Sai Vamsi Krishna Isukapalli, Probal Nag, and Sivaranjana Reddy Vennapusa. Cover image, volume 122, issue 12. *International Journal of Quantum Chemistry*, 122(12): e26714:1–e26714:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isukapalli:2022:OPO

[INV22b] Sai Vamsi Krishna Isukapalli, Probal Nag, and Sivaranjana Reddy Vennapusa. Optical properties of *para*-oligophenylenes: a case study of electronic absorption spectrum and relaxation dynamics of terphenyl. *International Journal of Quantum Chemistry*, 122(13):e26912:1–e26912:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ikot:2020:TQI

[IRA+20] Akpan N. Ikot, Gaotsiwe Joel Rampho, Precious O. Amadi, Uduakobong S. Okorie, Makagamathe J. Sithole, and Mantile L. Lekala. Theoretic quantum information entropies for the generalized hyperbolic potential. *International Journal of Quantum Chemistry*, 120(24):e26410:1–e26410:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irikura:2020:TSO

[Iri20] Karl K. Irikura. Thermochemical spin–orbit corrections for atomic platinum (Pt). *International Journal of Quantum Chemistry*, 120(2):e26074:1–e26074:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irikura:2021:TSO

[Iri21] Karl K. Irikura. Thermochemical spin–orbit corrections for platinum cation (Pt^+). *International Journal of Quantum Chemistry*, 121(4):e26448:1–e26448:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Izsak:2021:LST

[Izs21] Róbert Izsák. A local similarity transformed equation of motion approach for calculating excited states. *International Journal of Quantum Chemistry*, 121(3):e26327:1–e26327:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jahanbani:2020:TIC

[Jah20] Akbar Jahanbani. On topological indices of carbon nanocones and nanotori. *International Journal of Quantum Chemistry*, 120(6):e26082:1–e26082:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Janbazi:2020:STH

[JAZ+20] Mehdi Janbazi, Yavar T. Azar, Farhood Ziaie, Khashayar Ghandi, Chérif F. Matta, and Muhammad Shadman Lakmehsari. Structures, g-tensors, and hyperfine coupling constants of L-α-alanine radicals in radiation dosimetry: an ab initio molecular dynamics simulation study. *International Journal of Quantum Chemistry*, 120(12):e26211:1–e26211:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jana:2021:RSE

[JBPV21] Irina Jana, Suhita Basumallick, Sourav Pal, and Nayana Vaval. Resonance study: Effect of partial triples excitation using complex absorbing potential-based Fock-space multireference coupled cluster. *International Journal of Quantum Chemistry*, 121(17):e26738:1–e26738:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Joseph:2020:IPT

[JD20] Huiet V. Joseph and Wallace D. Derricotte. Intramolecular proton transfer in the isomerization of hydroxyacetone: Characterization based on reaction force analysis and the bond fragility spectrum. *International Journal of Quantum Chemistry*, 120(17):e26269:1–e26269:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Janjua:2022:CEE

[JHH+22] Muhammad Ramzan Saeed Ashraf Janjua, Muhammad Haroon, Riaz Hussain, Muhammad Usman, Muhammad Usman Khan, and Waqas Amber Gill. Computational engineering to enhance the photovoltaic by end-capped and bridging core alterations: Empowering the future with solar energy through synergistic effect in D-A materials. *International Journal of Quantum Chemistry*, 122(1):e26821:1–e26821:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeszenszki:2022:ICE

[JIFM22] Péter Jeszenszki, Robbie T. Ireland, Dávid Ferenc, and Edit Mátyus. On the inclusion of cusp effects in expectation values with explicitly correlated Gaussians. *International Journal of Quantum Chemistry*, 122(8):e26819:1–e26819:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jespersen:2021:BMC

[JJJM21] Malte F. Jespersen, Solvejg Jørgensen, Matthew S. Johnson, and Kurt V. Mikkelsen. Bypassing the multireference character of singlet molecular oxygen, part 1:1,4-cycloaddition. *International Journal of Quantum Chemistry*, 121

(6):e26523:1–e26523:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2020:VRD

[JMOW20] Kaili Jiang, Martín A. Mosquera, Yan Oueis, and Adam Wasserman. Virial relations in density embedding. *International Journal of Quantum Chemistry*, 120(21):e26204:1–e26204:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jana:2020:QST

[JPSC20] Gourhari Jana, Ranita Pal, Shamik Sural, and Pratim Kumar Chattaraj. Quantitative structure-toxicity relationship: an "in silico study" using electrophilicity and hydrophobicity as descriptors. *International Journal of Quantum Chemistry*, 120(6):e26097:1–e26097:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayasree:2021:CUM

[JRA21] Elambalassery G. Jayasree, Sobhana Reshma, and Mohanan Aswathy. Computationally unraveling the mechanism and selectivity of five and six membered N-heterocyclic carbene-catalyzed alkyne hydrochalcogenation. *International Journal of Quantum Chemistry*, 121(13):e26652:1–e26652:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorgensen:2021:BAP

[JS21] Maria W. Jørgensen and Stephan P. A. Sauer. Benchmarking anisotropic polarizabilities for 14 (hetero)-aromatic molecules at RPA, RPA(D), HRPA, HRPA(D), SOPPA, SOPPA(CC2), SOPPA(CCSD), CC2, CCSD and CC3 levels. *International Journal of Quantum Chemistry*, 121(9): e26593:1–e26593:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2021:MBH

[JSF+21] Shan Jiang, Lin Shao, Touwen Fan, Jia-Ming Duan, Xiao-Tao Chen, and Bi-Yu Tang. Mechanical behavior of high entropy carbide (HfTaZrTi)C and (HfTaZrNb)C under high pressure: Ab initio study. *International Journal of Quantum Chemistry*, 121(5):e26509:1–e26509:??, March 5, 2021.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jahanpanah:2022:RRV

[JVK22] Jafar Jahanpanah, A. Vahedi, and H. Khosrojerdi. Relativistic ro-vibrational feature of electron in Bohr's orbits of hydrogen-like atoms in Heisenberg picture. *International Journal of Quantum Chemistry*, 122(14):e26911:1–e26911:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jing:2020:CSP

[JWZZ20] Su-Hua Jing, Bin-Bin Wang, Xiao-Yun Zhou, and Ti-Xian Zeng. Comparative study of the photoassociation reaction of He + X^+ → HeX^+ (X = H, D): Including multiphoton transitions and dissociations. *International Journal of Quantum Chemistry*, 120(12):e26196:1–e26196:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2021:ISN

[JXL+21] Xinghui Jin, Menghui Xiao, Luhao Liu, Jianhua Zhou, and Bingcheng Hu. Investigation on a series of 3-nitro-1,2,4-triazol-5-one based energetic derivatives: Molecular design and screening. *International Journal of Quantum Chemistry*, 121(6):e26542:1–e26542:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorstad:2022:SCC

[JXM22] Jason V. Jorstad, Tian Xie, and Christine M. Morales. Δ-SCF calculations of core electron binding energies in first-row transition metal atoms. *International Journal of Quantum Chemistry*, 122(10):e26881:1–e26881:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2020:SMH

[JXYL20] Pingguo Jiang, Yiyu Xiao, Xiangbiao Yu, and Wenjie Liu. Study on mechanism of hydrogen adsorption on WO_3, $W_{20}O_{58}$, and $W_{18}O_{49}$. *International Journal of Quantum Chemistry*, 120(2):e26072:1–e26072:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2021:SST

[JZL+21] Xin Jiang, Zhenming Zhang, Diqiang Luo, Jinglin You, and Chaobin Lai. Structural stability and thermodynamic properties of $(Y_2O_3)_n$ (n = 1–15) clusters based on density functional theory. *International Journal of Quantum Chemistry*, 121(23):e26802:1–e26802:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2020:SME

[JZX+20] Diyou Jiang, Shuying Zhong, Wenbo Xiao, Desheng Liu, Musheng Wu, and Sanqiu Liu. Structural, mechanical, electronic, and thermodynamic properties of pure tungsten metal under different pressures: a first-principles study. *International Journal of Quantum Chemistry*, 120 (13):e26231:1–e26231:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2021:FPI

[KA21] Prabhleen Kaur and Md. Ehesan Ali. First principle investigations of long-range magnetic exchange interactions via polyacene couplers. *International Journal of Quantum Chemistry*, 121(20):e26756:1–e26756:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kirmani:2021:TIQ

[KAA21] Syed Ajaz K. Kirmani, Parvez Ali, and Faizul Azam. Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients. *International Journal of Quantum Chemistry*, 121(9): e26594:1–e26594:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kosar:2020:BAS

[KAG+20] Naveen Kosar, Khurshid Ayub, Mazhar A. Gilani, Faheem Shah, and Tariq Mahmood. Benchmark approach to search of cost-effective and accurate density functional for homolytic cleavage of C-Mg bond of Grignard reagent. *International Journal of Quantum Chemistry*, 120(4):e26106:1–e26106:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2021:FPE

[Kan21] Sung Gu Kang. First-principles exploration of $MgTi_2O_5$ and MgV_2O_5 for CO_2 capture and conversion. *International Journal of Quantum Chemistry*, 121(11):e26637:1–e26637:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2022:TIM

[Kan22] Sung Gu Kang. Theoretical investigation of metal oxides for SO_2 capture through first-principles calculations. *International Journal of Quantum Chemistry*, 122(1):e26822:1–e26822:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2021:PFD

[KAUB21] Gohar Zeb Khan, Imrana Ashraf, Arif Ullah, and Bakht Amin Bacha. Plasmon's Fizeau-dragging effect at the interface of atomic and nano-composites media. *International Journal of Quantum Chemistry*, 121(13):e26655:1–e26655:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kilic:2021:ORP

[KB21] Kadir Kiliç and Mustafa Kemal Bahar. Optical response of plasma processed quantum dot under the external fields. *International Journal of Quantum Chemistry*, 121 (7):e26564:1–e26564:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Bah22].

Kashyap:2020:COC

[KBR+20] Chayanika Kashyap, Indrani Baruah, Shahnaz S. Rohman, Sabnam S. Ullah, Amlan J. Kalita, Gargi Borgohain, and Ankur K. Guha. Carbonyl oxide chemistry in water cluster: an extended computational study. *International Journal of Quantum Chemistry*, 120(23):e26386:1–e26386:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalita:2022:VHS

[KDY+22] Amlan J. Kalita, Priyanka Dutta, Farnaz Yashmin, Ritam R. Borah, Rinu P. Deka, and Ankur K. Guha. Viability of half-sandwich complex of heavier group-14 elements (Si–Pb) with neutral Be_3 ring and its potential application as H_2 storage material. *International Journal of Quantum Chemistry*, 122(9):e26878:1–e26878:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karmakar:2020:LIE

[KGSD20] Shiladitya Karmakar, Debashree Ghosh, and Tanusri Saha-Dasgupta. Light-induced excited spin-state trapping in spin crossover model system. *International Journal of Quantum Chemistry*, 120(6):e26122:1–e26122:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2020:GPM

[KH20] Ashish Kumar and Manoj K. Harbola. A general penalty method for density-to-potential inversion. *International Journal of Quantum Chemistry*, 120(22):e26400:1–e26400:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khalil:2021:SVM

[KHH+21] R. M. Arif Khalil, Muhammad Iqbal Hussain, Fayyaz Hussain, Anwar Manzoor Rana, G. Murtaza, Muhammad Shakeel, and Hafiz M. Asif Javed. Structural, vibrational, mechanical, and optoelectronic properties of $LiBH_4$ for hydrogen storage and optoelectronic devices: First-principles study. *International Journal of Quantum Chemistry*, 121(4):e26444:1–e26444:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kheirabadi:2020:CMK

[KI20] Ramesh Kheirabadi and Mohammad Izadyar. Computational modeling of the kinetics and mechanism of tellurium-based glutathione peroxidase mimic. *International Journal of Quantum Chemistry*, 120(12):e26201:1–e26201:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kido:2021:TII

[Kid21] Kentaro Kido. A theoretical investigation on the intermolecular potential curve between ruthenium tetroxide and NO_X

(X = 1, 2). *International Journal of Quantum Chemistry*, 121(21):e26781:1–e26781:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2021:DCB

[KJA+21] Memoona Khan, Faiza Jilani, Amna Ayub, Zubera Naseem, Ali Raza Ayub, Muhammad Shabir Mahr, and Javed Iqbal. Designing of cyanobenzene based small molecules with suitable photovoltaic parameters for organic solar cells. *International Journal of Quantum Chemistry*, 121(15):e26673:1–e26673:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kostjukova:2021:ESV

[KK21] Lyudmila O. Kostjukova and Victor V. Kostjukov. The electronic states and vibronic absorption spectrum of berberine in aqueous solution. *International Journal of Quantum Chemistry*, 121(6):e26537:1–e26537:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaledin:2021:ESA

[KKH21] Leonid A. Kaledin, Alexey L. Kaledin, and Michael C. Heaven. The electronic structure of the actinide oxides and their singly and doubly charged cations: a ligand field approach. *International Journal of Quantum Chemistry*, 121 (8):e26588:1–e26588:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Konig:2021:GFT

[KKRR21] Carolin König, Vera Krewald, Michael Roemelt, and Mariana Rossi. Germany's future in theoretical and computational chemistry: a special issue celebrating DEAL. *International Journal of Quantum Chemistry*, 121(3):e26587:1–e26587:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kostjukova:2021:TDA

[KLK21] Lyudmila O. Kostjukova, Svetlana V. Leontieva, and Victor V. Kostjukov. TD-DFT absorption spectrum of Azure A in aqueous solution: Vibronic transitions and electronic properties. *International Journal of Quantum Chem-*

istry, 121(14):e26662:1–e26662:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khrenova:2021:BSH

[KLT21] Maria G. Khrenova, Elena O. Levina, and Vladimir G. Tsirelson. Benchmark studies of hydrogen bond governing reactivity of cephalosporins in L1 metallo-β-lactamase: Efficient and reliable QSPR equations. *International Journal of Quantum Chemistry*, 121(4):e26451:1–e26451:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koch:2021:CDT

[KM21a] Daniel Koch and Sergei Manzhos. Can doping of transition metal oxide cathode materials increase achievable voltages with multivalent metals? *International Journal of Quantum Chemistry*, 121(2):e26439:1–e26439:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2021:EST

[KM21b] Rahul Kumar and Dilip Kumar Maity. End-substituted thiahelicenes for electronic device applications. *International Journal of Quantum Chemistry*, 121(4):e26450:1–e26450:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2022:IME

[KMG22] Pradeep Kumar, Shabir Ahmad Mir, and Dinesh C. Gupta. Investigating the magneto-electronic, structural, mechanical, and thermodynamic properties of filled skutterudite $NdRu_4Sb_{12}$ and $EuRu_4Sb_{12}$: a first-principles perspective. *International Journal of Quantum Chemistry*, 122(3): e26834:1–e26834:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2020:DSC

[KMH+20] Muhammad Usman Khan, Muhammad Yasir Mehboob, Riaz Hussain, Zainab Afzal, Muhammad Khalid, and Muhammad Adnan. Designing spirobifullerene core based three-dimensional cross shape acceptor materials with promising photovoltaic properties for high-efficiency organic solar cells. *International Journal of Quantum Chemistry*, 120(22):e26377:1–e26377:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kapusta:2021:KET

[KMK21] Dmitry P. Kapusta, Fedor D. Mulashkin, and Maria G. Khrenova. Keto-enol tautomerism of the 4,5-dimethyl-2-(2'-hydroxyphenyl)imidazole in water solution: Modeling equilibrium between neutral forms and accurate assignment of the absorption bands. *International Journal of Quantum Chemistry*, 121(8):e26577:1–e26577:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2020:CCN

[KOB20] Douglas J. Klein, Yenni P. Ortiz, and Laimutis Bytautas. Conjugated-carbon nanostructures: Emergences. *International Journal of Quantum Chemistry*, 120(22):e26367:1–e26367:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Konig:2021:TMA

[Kön21] Carolin König. Tailored multilevel approaches in vibrational structure theory: a route to quantum mechanical vibrational spectra for complex systems. *International Journal of Quantum Chemistry*, 121(3):e26375:1–e26375:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kovacs:2020:SBL

[Kov20] Attila Kovács. Structure and bonding of lanthanide dinitrogen complexes, $Ln(N_2)_{1-8}$. *International Journal of Quantum Chemistry*, 120(1):e26051:1–e26051:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2020:ABL

[KRB20] Naveen Kumar, Prashant Raj, and Pananghat Balanarayan. Atop-the-barrier localization in periodically driven double wells: a minimization of information entropic sums in conjugate spaces. *International Journal of Quantum Chemistry*, 120(7):e26137:1–e26137:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalita:2021:SSP

[KRK+21] Amlan J. Kalita, Shahnaz S. Rohman, Chayanika Kashyap, Sabnam S. Ullah, Indrani Baruah, Lakhya J. Mazumder, and Ankur K. Guha. In silico search for planar hexacoordinate silicon atom: a kinetically viable species. *International Journal of Quantum Chemistry*, 121(14):e2664:1–e2664:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kashinski:2021:DFT

[KRS+21] David O. Kashinski, Tyler J. Radziewicz, Matthew G. Suarez, Constantine C. Stephens, and Edward F. C. Byrd. Density functional theory calculation of the Renner–Teller effect in NCO: Preliminary assessment of exact exchange energy on the accuracy of the $X^2\Pi$ Renner coefficient. *International Journal of Quantum Chemistry*, 121(23):e26804:1–e26804:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuzmin:2021:CNB

[KS21] Anton V. Kuzmin and Bagrat A. Shainyan. Carbon nanotube-based titanium- and zirconium-doped [M-N_4] type ORR catalysts. First principle study. *International Journal of Quantum Chemistry*, 121(24):e26809:1–e26809:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kowalewski:2022:SPQ

[KS22] Markus Kowalewski and Phillip Seeber. Sustainable packaging of quantum chemistry software with the Nix package manager. *International Journal of Quantum Chemistry*, 122(9):e26872:1–e26872:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kolar:2020:ASR

[KSP20] Michal H. Kolár, Denisa Suchá, and Michal Pitonák. Assessment of scalar relativistic effects on halogen bonding and σ-hole properties. *International Journal of Quantum Chemistry*, 120(23):e26392:1–e26392:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khalili:2021:CMC

[KVCS21] Fatemeh Khalili, Mohsen Vafaee, Daeheum Cho, and Babak Shokri. Charge migration in caffeine: a real-time time-dependent density functional theory study. *International Journal of Quantum Chemistry*, 121(19):e26754:1–e26754:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2020:TIS

[KWWZ20] Juanxia Kang, Yongcheng Wang, Jingjing Wu, and Zhiming Zhu. Theoretical investigations of spin–orbit coupling and intersystem crossing in reaction carbon dioxide activated by $[Re(CO)_2]^+$. *International Journal of Quantum Chemistry*, 120(5):e26109:1–e26109:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koh:2020:GGS

[KYL+20] Pin W. Koh, Tiem L. Yoon, Thong L. Lim, Yee H. R. Chang, and Eong S. Goh. Generation of ground-state structures and electronic properties of ternary Al_x Ti_y Ni_z clusters $(x + y + z = 6)$ with a two-stage density functional theory global search approach. *International Journal of Quantum Chemistry*, 120(2):e26079:1–e26079:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kacka-Zych:2021:UUS

[KZ21] Agnieszka Kacka-Zych. Understanding the uniqueness of the stepwise $[4 + 1]$ cycloaddition reaction between conjugated nitroalkenes and electrophilic carbene systems with a molecular electron density theory perspective. *International Journal of Quantum Chemistry*, 121(2):e26440:1–e26440:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:DBB

[LAAP21] Jia-Bao Liu, Micheal Arockiaraj, M. Arulperumjothi, and Savari Prabhu. Distance based and bond additive topological indices of certain repurposed antiviral drug compounds tested for treating COVID-19. *International Journal of Quantum Chemistry*, 121(10):e26617:1–e26617:??, May 15,

2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lantz:2021:DLI

[LACP21] Victor Lantz, Najmeh Abiri, Gillis Carlsson, and Mats-Erik Pistol. Deep learning for inverse problems in quantum mechanics. *International Journal of Quantum Chemistry*, 121 (9):e26599:1–e26599:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:EUS

[LAKJ20] Shuman Li, Alireza Azizi, Steven R. Kirk, and Samantha Jenkins. An explanation of the unusual strength of the hydrogen bond in small water clusters. *International Journal of Quantum Chemistry*, 120(19):e26361:1–e26361:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzon:2020:OTB

[LBG20] Álvaro Luzón, Enrique Buendía, and Francisco J. Gálvez. One and two body densities for excited states of the helium confined atom. *International Journal of Quantum Chemistry*, 120(1):e26048:1–e26048:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laestadius:2020:UCM

[LBP20] Andre Laestadius, Michael Benedicks, and Markus Penz. Unique continuation for the magnetic Schrödinger equation. *International Journal of Quantum Chemistry*, 120(8): e26149:1–e26149:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lanza:2020:WMA

[LC20] Giuseppe Lanza and Maria A. Chiacchio. The water molecule arrangement over the side chain of some aliphatic amino acids: a quantum chemical and bottom-up investigation. *International Journal of Quantum Chemistry*, 120(9): e26161:1–e26161:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Littlefair:2021:AFE

[LCP21] Josh D. Littlefair, Daniel J. Cole, and Thomas J. Penfold. On assessing functional errors in density functional theory using atomisation energies and electric field gradients. *International Journal of Quantum Chemistry*, 121(23):e26799:1–e26799:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:MSI

[LCX+21] Hechao Liu, Hanlin Chen, Qiqi Xiao, Xiaona Fang, and Zikai Tang. More on Sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 121(17):e26689:1–e26689:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Fernandez:2020:DOS

[LFMG20] José L. López-Fernández, Ricardo A. Mosquera, and Ana M. Graña. Do one-step mechanisms always involve simultaneous evolution of electron density? QTAIM/IQA analysis of the Curtius rearrangement. *International Journal of Quantum Chemistry*, 120(10):e26170:1–e26170:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Linares-Flores:2020:RDA

[LFRTRP+20] Cristian Linares-Flores, Rodrigo Ramirez-Tagle, Macarena Rojas-Poblete, Ramiro Arratia-Perez, Alvaro Muñoz-Castro, and Raul Guajardo-Maturana. Role of donor-acceptor functional groups in N_3P_3 cyclic-triphosphazene backbone. Unraveling bonding characteristics from natural orbitals within an extended transition state-natural orbital for the chemical valence scheme. *International Journal of Quantum Chemistry*, 120(1):e26057:1–e26057:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:GSP

[LFX+21] Qin Liu, Chengbin Fu, Bo Xiao, Yanchun Li, Jianbo Cheng, Zhenbo Liu, Xin Yang, Xiufeng Xu, Hongtao Cui, and Qingzhong Li. Graphitic SiC: a potential anode material for Na-ion battery with extremely high storage capacity. *International Journal of Quantum Chemistry*, 121(10):e26608:1–e26608:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:TMS

[LG21] Jing Li and Wei Guan. Theoretical mechanistic study of nickel-catalyzed anti-Markovnikov hydroarylation of alkenes. *International Journal of Quantum Chemistry*, 121 (11):e26621:1–e26621:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:FPI

[LHL+21] Lili Liu, Lei Hu, Shanshan Liu, Jing Xiong, Qin Liao, and Yufeng Wen. First-principles investigations on the ground-state bulk properties and lattice constant dependent half-metallic ferrimagnetism of Mn_2NbSi full-Heusler compound. *International Journal of Quantum Chemistry*, 121 (7):e26566:1–e26566:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2020:TSC

[LK20] Kyungeon Lee and Dongwook Kim. A theoretical study of carbazole dimers: Does carbazole form an excimer that undermines the performance of organic light emitting diodes? *International Journal of Quantum Chemistry*, 120(19):e26363:1–e26363:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:DFTb

[LK21] Junqing Li and Lihua Kang. The density functional theory study of 2D nonmetallic catalyst defective graphene for acetylene hydration. *International Journal of Quantum Chemistry*, 121(7):e26561:1–e26561:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2020:TMC

[LL20] Min-Hsien Liu and Chun-Chih Lin. Theoretical modeling of the chemical synthesis and detonation performance of polynitrocubane derivatives. *International Journal of Quantum Chemistry*, 120(5):e26117:1–e26117:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:CMH

[LL21] Na Liu and Qingzhong Li. Can metal halides be electron donors in σ-hole and π-hole tetrel bonds? Cooperativity with an alkaline-earth bond. *International Journal of Quantum Chemistry*, 121(20):e26771:1–e26771:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2020:MBT

[LLC20] Chun-Yaung Lu, Tsung-Yen Lee, and Chia-Chun Chou. Moving boundary truncated grid method: Multidimensional quantum dynamics. *International Journal of Quantum Chemistry*, 120(1):e26055:1–e26055:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:DSM

[LLLL20] Weiyi Li, Geng Leng, Caiqin Li, and Yajing Lyu. A DFT study on mechanisms of CO_2 coupling with propargylic alcohols using alkali carbonates. *International Journal of Quantum Chemistry*, 120(8):e26150:1–e26150:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2020:TIT

[LLMQ20] Nan Lu, Xiaozheng Lan, Chengxia Miao, and Ping Qian. Theoretical investigation on transformation of Cr(II) to Cr(V) complexes bearing tetra-N-heterocyclic carbene and group transfer reactivity. *International Journal of Quantum Chemistry*, 120(18):e26340:1–e26340:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2021:TIM

[LLQ$^+$21] Nan Lu, Hui Liang, Ping Qian, Xiaozheng Lan, and Chengxia Miao. Theoretical investigation on the mechanism and enantioselectivity of organocatalytic asymmetric Povarov reactions of anilines and aldehydes. *International Journal of Quantum Chemistry*, 121(8):e26574:1–e26574:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:DFTa

[LLW+21] Chunlan Li, Wensheng Liu, Juan Wang, Shuwei Yao, and Yunzhu Ma. A density functional theory study on the structure formation of Al(III) carboxylate complexes in aqueous aluminum sols. *International Journal of Quantum Chemistry*, 121(2):e26430:1–e26430:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:RAS

[LLZ+20] Xiaoyan Li, Jiabin Liu, Qiao-Chu Zhang, Wenjing Zhang, and Yu Lan. Reagent addition sequence and equivalent in *N*-heterocyclic carbene-catalyzed nonpolar inversion enable conversion from aldimine to benzoxazole. *International Journal of Quantum Chemistry*, 120(14):e26249:1–e26249:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:STE

[LLZC20] Shan-Shan Li, Xiao-Hong Li, Rui-Zhou Zhang, and Hong-Ling Cui. Strain-tunable electronic properties and optical properties of Hf_2CO_2 MXene. *International Journal of Quantum Chemistry*, 120(22):e26365:1–e26365:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lima:2021:ITP

[LMA21] Francisco Cleiton E. Lima, Allan R. P. Moreira, and Carlos Alberto S. Almeida. Information and thermodynamic properties of a non-Hermitian particle ensemble. *International Journal of Quantum Chemistry*, 121(12):e26645:1–e26645:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lima:2021:SPL

[LMMA21] Francisco Cleiton E. Lima, Allan R. P. Moreira, Laura E. S. Machado, and Carlos Alberto S. Almeida. Statistical properties of linear Majorana fermions. *International Journal of Quantum Chemistry*, 121(18):e26749:1–e26749:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lembinen:2020:CCL

[LNE+20] Meeri Lembinen, Ergo Nõmmiste, Heigo Ers, Borja Docampo-Álvarez, Jaanus Kruusma, Enn Lust, and Vladislav B. Ivanistsev. Calculation of core-level electron spectra of ionic liquids. *International Journal of Quantum Chemistry*, 120(14):e26247:1–e26247:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:CCB

[LNX+21] Zi Li, Xing Nie, Tianlv Xu, Shuman Li, Yong Yang, Herbert Früchtl, Tanja van Mourik, Steven R. Kirk, Martin J. Paterson, Yasuteru Shigeta, and Samantha Jenkins. Control of chirality, bond flexing and anharmonicity in an electric field. *International Journal of Quantum Chemistry*, 121(22): e26793:1–e26793:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lombardo:2021:TEA

[Lom21] Giuseppe Marcello Lombardo. Tsallis q-exponentials as atomic orbitals in two-electron systems. *International Journal of Quantum Chemistry*, 121(5):e26489:1–e26489:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2022:TIA

[LPH22] Jia-Bao Liu, Xin-Bei Peng, and Sakander Hayat. Topological index analysis of a class of networks analogous to alicyclic hydrocarbons and their derivatives. *International Journal of Quantum Chemistry*, 122(2):e26827:1–e26827:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:EKC

[LQZ+21] Shaoli Liu, Lingxi Qi, Zheng Zhang, Xuejie Hou, and Wenzuo Li. Effect of K on carbon adsorption and deposition on the Co(111) surface. *International Journal of Quantum Chemistry*, 121(24):e26812:1–e26812:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leonardi:2020:PFS

[LRG+20] Angelina Leonardi, Heather M. Ricker, Ariel G. Gale, Benjamin T. Ball, Tuguldur T. Odbadrakh, George C. Shields, and Juan G. Navea. Particle formation and surface processes on atmospheric aerosols: a review of applied quantum chemical calculations. *International Journal of Quantum Chemistry*, 120(20):e26350:1–e26350:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:TAL

[LS21] Jia-Bao Liu and Rosary Maria Singaraj. Topological analysis of para-line graph of Remdesivir used in the prevention of corona virus. *International Journal of Quantum Chemistry*, 121(22):e26778:1–e26778:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:TIC

[LSG21] Siman Li, Li Shi, and Wei Gao. Topological indices computing on random chain structures. *International Journal of Quantum Chemistry*, 121(8):e26589:1–e26589:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:PEP

[LSS+21] Chengwei Liu, Yun Shi, Yaning Shang, Xin Wang, Dan Liu, Bhekie B. Mamba, Alex T. Kuvarega, and Jianzhou Gui. Promoting effect of PdZn alloy for selective hydrogenation of 5-hydroxylmethylfurfural: an experimental and density functional theory study. *International Journal of Quantum Chemistry*, 121(6):e26545:1–e26545:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:RSN

[LWC+21] Cui-Mei Li, Di Wu, Wei Chen, Jia-Yuan Liu, Dan Yu, and Ying Li. On reactivity of superatom Be_8C with nucleophiles to produce hydrogen. *International Journal of Quantum Chemistry*, 121(22):e26794:1–e26794:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:SEE

[LWH+21] Lili Liu, Miao Wang, Lei Hu, Yufeng Wen, and Youchang Jiang. Structural, elastic, and electronic properties of MgB_2C_2 under pressure from first-principles calculations. *International Journal of Quantum Chemistry*, 121(2): e26442:1–e26442:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2021:CSR

[LWR21] Tao Liu, Ping Wang, and Hong Ren. Computational study on the Rh-catalyzed C–C activation of cyclopropanol to construct diketone or monoketone. *International Journal of Quantum Chemistry*, 121(2):e26438:1–e26438:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lei:2020:TRO

[LWW20] Xiaoyang Lei, Weina Wang, and Wenliang Wang. Theoretical reinvestigation of the ozonolysis mechanism of allyl alcohol. *International Journal of Quantum Chemistry*, 120(23): e26387:1–e26387:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2021:FPI

[LXWZ21] Ruihu Lu, Lixue Xia, Huan Wang, and Yan Zhao. First-principles investigations on the synergistic effect of N-dopant and lattice-strain for CO_2 reduction to CO on graphene. *International Journal of Quantum Chemistry*, 121 (6):e26535:1–e26535:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leng:2021:TIS

[LXZ+21a] Jiancai Leng, Juntao Xin, Hong Zhou, Kan Li, Wei Hu, and Yujin Zhang. Theoretical insights into sensing performances of rhodamine-contained two-photon fluorescent probes for mercury ion. *International Journal of Quantum Chemistry*, 121(2):e26435:1–e26435:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2021:SLE

[LXZ21b] Hongyan Lu, Nini Xue, and Zhongxun Zhu. On the signless Laplacian Estrada index of uniform hypergraphs. *Inter-*

national Journal of Quantum Chemistry*, 121(8):e26579:1–e26579:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2021:OTT

[LYFL21] Wenshui Lin, Zhangyong Yan, Peifang Fu, and Jia-Bao Liu. Ordering trees by their ABC spectral radii. *International Journal of Quantum Chemistry*, 121(5):e26519:1–e26519:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2020:HFH

[LYT+20] Yidan Liu, Yizhong Yuan, Xiaohui Tian, Jianyong Yuan, and Jinyu Sun. High first-hyperpolarizabilities of thiobarbituric acid derivative-based donor-π-acceptor nonlinear optical-phores: Multiple theoretical investigations of substituents and conjugated bridges effect. *International Journal of Quantum Chemistry*, 120(10):e26176:1–e26176:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2020:TIR

[LYTS20] Yidan Liu, Yizhong Yuan, Xiaohui Tian, and Jinyu Sun. Theoretical investigation on reverse intersystem crossing from upper triplet to lowest singlet: a “hot exciton” path for blue fluorescent OLEDs. *International Journal of Quantum Chemistry*, 120(23):e26399:1–e26399:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2020:TCX

[LYW+20] Yu-Liang Liu, Chuan-Lu Yang, Mei-Shan Wang, Xiao-Guang Ma, and You-Gen Yi. Ternary chalcogenides $XGaS_2$ (X = Ag or Cu) for photocatalytic hydrogen generation from water splitting under irradiation of visible light. *International Journal of Quantum Chemistry*, 120(10):e26166:1–e26166:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2020:PHT

[LZ20] Xiaorui Liu and Min Zhang. Promising hole-transporting materials for perovskite solar cells: Modulation of the electron-deficient units in triphenylamine derivative-based molecules. *International Journal of Quantum Chemistry*, 120(2):e26070:1–e26070:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2021:DSN

[LZ21] Yan Li and Zhiqiang Zhang. A DFT study on NHC-catalyzed [4 + 2] annulation of 2H-azirines with ketones: Mechanism and selectivity. *International Journal of Quantum Chemistry*, 121(7):e26557:1–e26557:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2021:CEH

[LZL+21] Yousong Lu, Tianlei Zhang, Makroni Lily, Weina Wang, Fengyi Liu, and Wenliang Wang. The catalytic effects of H_2O, basic and acidic catalysts on the gas-phase hydrolysis mechanism of carbonyl fluoride (CF_2O). *International Journal of Quantum Chemistry*, 121(13):e26657:1–e26657:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lancheros:2020:MRR

[LZS20] Andres Lancheros, Ximena Zarate, and Eduardo Schott. Magnetic response and its relation to the keto-enol tautomerism of 3,3'-(1,4-phenylene)bis(pentane-2,4-dione): Experimental and theoretical insights. *International Journal of Quantum Chemistry*, 120(19):e26360:1–e26360:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:SNL

[LZSA20] Qishun Li, Shahid Zaman, Wanting Sun, and Jawad Alam. Study on the normalized Laplacian of a penta-graphene with applications. *International Journal of Quantum Chemistry*, 120(9):e26154:1–e26154:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2020:TEV

[LZZ+20] Kan Luo, Xian-Hu Zha, Yuhong Zhou, Qing Huang, Shenghu Zhou, and Shiyu Du. Theoretical exploration on the vibrational and mechanical properties of M_3 C_2 /M_3 C_2 T_2 MXenes. *International Journal of Quantum Chemistry*, 120(24):e26409:1–e26409:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez-Aguilar:2021:SFO

[MAHRA+21] Espiridión Martínez-Aguilar, H'Linh Hmok, Jordi Ribas-Ariño, Jesús María Siqueiros Beltrones, and Rosendo Lozada-Morales. Structural, ferroelectric, and optical properties of Bi^{3+} doped $YFeO_3$: a first-principles study. *International Journal of Quantum Chemistry*, 121(7):e26551:1–e26551:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mushtaq:2022:CMI

[MAK+22] Shagufa Mushtaq, Micheal Arockiaraj, Sandi Klavzar, J. Celin Fiona, and Krishnan Balasubramanian. Comment on Mostar indices of SiO_2 nanostructures and melem chain nanostructures. *International Journal of Quantum Chemistry*, 122(11):e26894:1–e26894:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Momen:2022:DTS

[MAMB+22] Roya Momen, Alireza Azizi, Alejandro Morales-Bayuelo, Mehdi Pazhoohesh, and Xiaobo Ji. Discerning torquoselectivity in a series of cyclobutene ring-opening reactions using quantum theory of atoms in molecules and stress tensor. *International Journal of Quantum Chemistry*, 122(2): e26826:1–e26826:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2021:FPSa

[MBKA21] Abdul Majid, Amber Batool, Salah Ud-Din Khan, and Ashfaq Ahmad. First-principles study of f-orbital-dependent band topology of topological rare earth hexaborides. *International Journal of Quantum Chemistry*, 121(4):e26452:1–e26452:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morsli:2021:SEE

[MBM+21] Amaria Morsli, Ali Bentouaf, Benzerdjab Amina Mahdad, Ibrahim Ameri, Mohammed Ameri, and Brahim Aïssa. Structural, electronic, elastic, magnetic and thermodynamic properties of Mn_2LuZ (Z = B, Al, Ga and In) Heusler compounds: a first-principle study. *International Journal* *of Quantum Chemistry*, 121(9):e26601:1–e26601:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maksimov:2021:CSF

[MBR21a] Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi. The conformational space of a flexible amino acid at metallic surfaces. *International Journal of Quantum Chemistry*, 121(3):e26369:1–e26369:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maksimov:2021:CIV

[MBR21b] Dmitrii Maksimov, Carsten Baldauf, and Mariana Rossi. Cover image, volume 121, issue 3. *International Journal of Quantum Chemistry*, 121(3):e26284:1–e26284:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malloum:2022:PES

[MC22] Alhadji Malloum and Jeanet Conradie. Potential energy surface of the thiophene pentamer and non-covalent interactions. *International Journal of Quantum Chemistry*, 122(4): e26840:1–e26840:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marques:2020:EVH

[MCP+20] Suélio Marques, Marcos A. Castro, Renato B. Pontes, Salviano A. Leão, and Tertius L. Fonseca. Electronic and vibrational hyperpolarizabilities of alkali- and alkaline-earth-doped boron nitride nanotubes. *International Journal of Quantum Chemistry*, 120(3):e26093:1–e26093:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhammady:2020:ISE

[MEWD20] Shibghatullah Muhammady, Adelya S. Erlyanti, Rena Widita, and Yudi Darma. Investigation of structural and electronic properties by pnictogen substitution in the layered oxypnictides (LaO)Zn Pn (Pn = P, As, Sb). *International Journal of Quantum Chemistry*, 120(3):e26090:1–e26090:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez-Flores:2021:ITH

[MF21a] César Martínez-Flores. The information theory of the helium atom in screened Coulomb potentials. *International Journal of Quantum Chemistry*, 121(6):e26529:1–e26529:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins:2021:RSP

[MF21b] Francisco A. Martins and Matheus P. Freitas. Regio and stereochemical probes of iodine interactions in diiodocyclododecanes. *International Journal of Quantum Chemistry*, 121(17):e26739:1–e26739:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malloum:2020:BEI

[MFC20a] Alhadji Malloum, Jean J. Fifen, and Jeanet Conradie. Binding energies and isomer distribution of neutral acetonitrile clusters. *International Journal of Quantum Chemistry*, 120 (13):e26221:1–e26221:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malloum:2020:TIS

[MFC20b] Alhadji Malloum, Jean J. Fifen, and Jeanet Conradie. Theoretical infrared spectrum of the ethanol hexamer. *International Journal of Quantum Chemistry*, 120(13):e26234:1–e26234:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mihalovits:2022:RQC

[MFK22] Levente M. Mihalovits, György G. Ferenczy, and György M. Keserü. The role of quantum chemistry in covalent inhibitor design. *International Journal of Quantum Chemistry*, 122 (8):e26768:1–e26768:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2020:SEV

[MHD20] Madhubani Mukherjee, Soumi Haldar, and Achintya K. Dutta. Solvation effect on the vertical ionization energy of adenine-thymine base pair: From microhydration to bulk. *International Journal of Quantum Chemistry*, 120 (6):e26127:1–e26127:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moradi:2021:FPS

[MHS21] Zahra Moradi, Amir Heydarinasab, and Farshid Pajoum Shariati. First-principle study of doping effects (Ti, Cu, and Zn) on electrochemical performance of Li_2MnO_3 cathode materials for lithium-ion batteries. *International Journal of Quantum Chemistry*, 121(4):e26458:1–e26458:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mehranfar:2020:TSA

[MI20] Aliyeh Mehranfar and Mohammad Izadyar. Theoretical study on alkaloid encapsulating via cyclopentanocucurbit[n]uril ($n = 8, 10$) /graphene oxide heterojunction. *International Journal of Quantum Chemistry*, 120(9): e26155:1–e26155:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Momin:2021:ISE

[MIM21] Md. Abdul Momin, Md. Aminul Islam, and Abhijit Majumdar. Influence on structural, electronic and optical properties of Fe doped ZnS quantum dot: a density functional theory based study. *International Journal of Quantum Chemistry*, 121(21):e26786:1–e26786:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2020:QCS

[MJA20] Tianxiao Ma, Chao Jin, and Saeed Amir Aslanzadeh. Quantum chemical study on the sensing properties of Pt-decorated BC_3 nanotube toward metronidazole drug. *International Journal of Quantum Chemistry*, 120(24):e26407:1–e26407:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosquera:2020:QEM

[MJRS20] Martín A. Mosquera, Leighton O. Jones, Mark A. Ratner, and George C. Schatz. Quantum embedding for material chemistry based on domain separation and open subsystems. *International Journal of Quantum Chemistry*, 120(21):e26184:1–e26184:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mittal:2021:TAS

[MK21] Ankit Mittal and Rita Kakkar. A theoretical assessment of the structural and electronic features of some retrochalcones. *International Journal of Quantum Chemistry*, 121 (24):e26797:1–e26797:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mkadmh:2020:DCD

[Mka20] Ahmed M. Mkadmh. DFT and CIS(D) theoretical study on the ground and excited states of pentanitrogen cation. *International Journal of Quantum Chemistry*, 120(23):e26393:1–e26393:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mirzaie-Khalilabadi:2021:INC

[MKD21] Elahe Mirzaie-Khalilabadi and Maryam Dehestani. Investigation of nonadiabatic coupling and diabatic electronic population dynamics on F_2O^+ cation within multi reference configuration interaction calculations. *International Journal of Quantum Chemistry*, 121(15):e26675:1–e26675:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2021:DSS

[MKKA21] Abdul Majid, Hajra Kanwal, Salah Ud-Din Khan, and Ashfaq Ahmad. A DFT study of structural and thermal properties of 2D layers. *International Journal of Quantum Chemistry*, 121(11):e26625:1–e26625:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2022:DFT

[MKKK22] Abdul Majid, Hajra Kanwal, Salahuddin Khan, and Shaukat Khan. A density functional theory study of electronic properties of transition metals doped silicon carbide monolayer. *International Journal of Quantum Chemistry*, 122(9):e26877:1–e26877:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melchakova:2020:EEF

[MKM+20] Iuliia Melchakova, Evgenia A. Kovaleva, Natalia S. Mikhaleva, Felix N. Tomilin, Sergey G. Ovchinnikov, Alexander A.

Kuzubov, and Paul Avramov. External electric field effect on electronic properties and charge transfer in CoI_2 / NiI_2 spinterface. *International Journal of Quantum Chemistry*, 120(3):e26092:1–e26092:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2022:EPS

[MKuAS+22] Abdul Majid, Saba Kiran, Qurat ul Ain Sandhu, Salahuddin Khan, and Shaukat Khan. The effects of polar solvents on structural, electronic, and optical properties of organic dyes. *International Journal of Quantum Chemistry*, 122(9): e26876:1–e26876:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2020:APA

[MM20] Rintu Mondal and Debasis Mukhopadhyay. On the aspect of plane of appearance of Jahn–Teller and Renner–Teller intersections in tetra-atomic system- a case study with $HCNO^+$. *International Journal of Quantum Chemistry*, 120 (11):e26195:1–e26195:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2021:SNA

[MM21] Rintu Mondal and Debasis Mukhopadhyay. Study of nonadiabatic interactions among low-lying electronic states of HeH_2^+ with its implication in its dissociation into various species. *International Journal of Quantum Chemistry*, 121 (7):e26552:1–e26552:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manogaran:2022:ACF

[MM22a] Dhivya Manogaran and Sadasivam Manogaran. Anharmonicity in compliance formalism: Potential constants and interaction coordinates. *International Journal of Quantum Chemistry*, 122(4):e26841:1–e26841:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matta:2022:CIV

[MM22b] Chérif F. Matta and Lou Massa. Cover image, volume 122, issue 4. *International Journal of Quantum Chemistry*, 122(4):e26698:1–e26698:??, February 15, 2022. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matta:2022:TPT

[MM22c] Chérif F. Matta and Lou Massa. Two projector triple products in quantum crystallography. *International Journal of Quantum Chemistry*, 122(4):e26838:1–e26838:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendez:2016:DIM

[MMM16] Alejandra M. P. Mendez, Darío M. Mitnik, and Jorge E. Miraglia. Depurated inversion method for orbital-specific exchange potentials. *International Journal of Quantum Chemistry*, 116(24):1882–1890, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Cin20] and reply [MMM20].

Mitnik:2020:RCD

[MMM20] D. M. Mitnik, A. M. P. Mendez, and J. E. Miraglia. Reply to "Comment on 'Depurated Inversion Method for Orbital-Specific Exchange Potentials'". *International Journal of Quantum Chemistry*, 120(4):e26102:1–e26102:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Cin20].

McDonald:2020:BCU

[MNN+20] Ashley Ringer McDonald, Jessica A. Nash, Paul S. Nerenberg, K. Aurelia Ball, Olaseni Sode, Jonathon J. Foley IV, Theresa L. Windus, and T. Daniel Crawford. Building capacity for undergraduate education and training in computational molecular science: a collaboration between the MERCURY consortium and the Molecular Sciences Software Institute. *International Journal of Quantum Chemistry*, 120(20):e26359:1–e26359:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhammady:2020:FSD

[MNWD20] Shibghatullah Muhammady, Fatimah A. Noor, Rena Widita, and Yudi Darma. Ferromagnetism and structural deformation in monolayer alpha lead oxide induced by N and F doping: New insights from first principles. *International Journal of Quantum Chemistry*, 120(16):e26268:1–e26268:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monu:2021:SEP

[MOB21] Monu, Binod Kumar Oram, and Biman Bandyopadhyay. Simultaneous exhibition of positive and negative cooperativity by purely C– H$\cdots$OH-bonded (1,3-cyclohexanedione)$_n$ (n = 2–6) clusters: a density functional theoretical investigation. *International Journal of Quantum Chemistry*, 121 (8):e26581:1–e26581:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mokkath:2021:OFL

[Mok21a] Junais Habeeb Mokkath. Optical features of ligated semiconducting quantum dots subjected to an electric field. *International Journal of Quantum Chemistry*, 121(20): e26763:1–e26763:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mokkath:2021:PPN

[Mok21b] Junais Habeeb Mokkath. Plasmonic properties of nanohybrids made of metallic nanoring and benzene molecules. *International Journal of Quantum Chemistry*, 121(12): e26646:1–e26646:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mokkath:2021:SCD

[Mok21c] Junais Habeeb Mokkath. Subfemtosecond charge dynamics in vertically stacked bilayer silicene. *International Journal of Quantum Chemistry*, 121(6):e26521:1–e26521:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mostafanejad:2021:FPQ

[Mos21] Mohammad Mostafanejad. Fractional paradigms in quantum chemistry. *International Journal of Quantum Chemistry*, 121(20):e26762:1–e26762:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgante:2020:DDT

[MP20] Pierpaolo Morgante and Roberto Peverati. The devil in the details: a tutorial review on some undervalued aspects of density functional theory calculations. *International Journal of Quantum Chemistry*, 120(18):e26332:1–e26332:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majumdar:2021:DFS

[MR21] Sangita Majumdar and Amlan K. Roy. Density functional study of atoms spatially confined inside a hard sphere. *International Journal of Quantum Chemistry*, 121(11):e26630:1–e26630:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matulis:2020:ATP

[MRI20] Vitaly E. Matulis, Ekaterina G. Ragoyja, and Oleg A. Ivashkevich. Accurate theoretical prediction of optical properties of BODIPY dyes. *International Journal of Quantum Chemistry*, 120(9):e26159:1–e26159:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manzoor:2022:CEM

[MSA22] Shazia Manzoor, Muhammad Kamran Siddiqui, and Sarfraz Ahmad. Computation of entropy measures for phthalocyanines and porphyrins dendrimers. *International Journal of Quantum Chemistry*, 122(5):e26854:1–e26854:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohammad-Salim:2021:MED

[MSADA21] Haydar A. Mohammad-Salim, Nivedita Acharjee, Luis R. Domingo, and Hassan H. Abdallah. A molecular electron density theory study for [3 + 2] cycloaddition reactions of 1-pyrroline-1-oxide with disubstituted acetylenes leading to bicyclic 4-isoxazolines. *International Journal of Quantum Chemistry*, 121(5):e26503:1–e26503:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2020:TDD

[MSKA20] Abdul Majid, Maryam Sana, Salah Ud-Din Khan, and Naeem Ahmad. Time-dependent density functional theory investigations on structural modification in carbazole-based organic photosensitizers to improve electron injection in dye-sensitized solar cell. *International Journal of Quantum Chemistry*, 120(15):e26253:1–e26253:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2021:FPSb

[MSKA21] Abdul Majid, Maryam Sana, Salah Ud-Din Khan, and Ashfaq Ahmad. A first-principles study on improvement of photoinjection in organic dyes. *International Journal of Quantum Chemistry*, 121(9):e26596:1–e26596:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2020:TIS

[MSM+20] Nana Ma, Mengxiao Song, Qi Meng, Changgeng Wei, and Guisheng Zhang. Theoretical insight into the solvent effect on the stoichiometric reduction of carbonyl compounds by ammonia borane and N -methyl amine borane. *International Journal of Quantum Chemistry*, 120(9):e26162:1–e26162:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manonmani:2020:HHP

[MSS20] Gunasekaran Manonmani, Lakshmanan Sandhiya, and Kittusamy Senthilkumar. Hydrolysis of $HNSO_2$: a potential route for atmospheric production of H_2 SO_4 and NH_3. *International Journal of Quantum Chemistry*, 120(11):e26182:1–e26182:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mahato:2022:FRS

[MSS22] Dibyendu Mahato, Lalita Sharma, and Rajesh Srivastava. Fully relativistic study on electron impact elastic scattering from N^{q+} ($q = 1$—3), Na^+, Ar^{q+} ($q = 1$—3, 7–8), and Xe^{q+} (q = 2–6, 8). *International Journal of Quantum Chemistry*, 122(1):e26815:1–e26815:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mubarak:2021:IPP

[MT21] Ahmad A. Mubarak and Saad Tariq. Influence of pressure on piezoelectric, polarizing, and magnetic nature of $SmFeO_3$: A DFT study. *International Journal of Quantum Chemistry*, 121(4):e26471:1–e26471:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mubarak:2022:EEV

[MTA+22] A. A. Mubarak, Saad Tariq, B. O. Alsobhi, Farida Hamioud, and Ayash O. Alrashdi. Elucidating the effect of V_x doped $LaFe_{1-x}O_3$ for advanced optical, spintronic, and thermoelectric devices. *International Journal of Quantum Chemistry*, 122(5):e26850:1–e26850:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marjollet:2021:SSC

[MW21] Adrien Marjollet and Ralph Welsch. State-selective cross sections from ring polymer molecular dynamics. *International Journal of Quantum Chemistry*, 121(3):e26447:1–e26447:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendoza-Wilson:2020:IBP

[MWBQ20] Ana M. Mendoza-Wilson and René R. Balandrán-Quintana. Interactions between procyanidin oligomers and the active form of matrix metalloproteinase-7: a theoretical insight. *International Journal of Quantum Chemistry*, 120(19): e26349:1–e26349:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2021:TDB

[MWC+21] Jingwei Meng, Chenglong Wang, Minghua Cheng, Shuhai Zhang, Ruijun Gou, Yahong Chen, and Yang Li. The thermal decomposition behavior of the TNT-RDX-Al explosive by molecular kinetic simulation. *International Journal of Quantum Chemistry*, 121(11):e26635:1–e26635:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moghadam:2021:PNR

[MZ21] Maryam Manafi Moghadam and Mehdi Zamani. Performance of NO_2 -rich multifunctionalized C_{60} derivatives as new high-energy-density nanomaterials. *International Journal of Quantum Chemistry*, 121(5):e26504:1–e26504:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2020:ASC

[MZD+20] Di Ma, Jing Zhang, Yaxin Di, Jianfeng Wang, Shaokang Guan, and Tao Zhang. Atomic structure of $Co_{92-x}B_xTa_8$ glassy alloys studied by ab initio molecular dynamics simulations. *International Journal of Quantum Chemistry*, 120(23):e26406:1–e26406:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mao:2021:AAB

[MZF21] Xiaotong Mao, Lin Zhu, and Aiping Fu. Arsenene, antimonene and bismuthene as anchoring materials for lithium-sulfur batteries: a computational study. *International Journal of Quantum Chemistry*, 121(14):e26661:1–e26661:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosyagin:2020:GRE

[MZT20] Nikolai S. Mosyagin, Andrei V. Zaitsevskii, and Anatoly V. Titov. Generalized relativistic effective core potentials for superheavy elements. *International Journal of Quantum Chemistry*, 120(2):e26076:1–e26076:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2021:BPC

[MZXL21] Fenfen Ma, Xiaoyan Zheng, Jing Xie, and Zesheng Li. Binding properties of cucurbit[7]uril to neutral and protonated amino acids: a theoretical study. *International Journal of Quantum Chemistry*, 121(5):e26491:1–e26491:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2021:CFI

[NACP21] João P. G. Nascimento, Vanderley Aguiar, Raimundo N. Costa Filho, and João Milton Pereira, Jr. Comment on “Fisher information of a vector potential for time-dependent Feinberg–Horodecki equation”. *International Journal of Quantum Chemistry*, 121(12):e26629:1–e26629:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [OO21a, OO21b].

Nagan:2020:ULW

[Nag20a] Maria C. Nagan. Using a lab wiki for longevity and knowledge transfer in undergraduate research. *International Journal of Quantum Chemistry*, 120(20):e26262:1–e26262:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2020:RIE

[Nag20b] Ágnes Nagy. Relative information in excited-state orbital-free density functional theory. *International Journal of Quantum Chemistry*, 120(23):e26405:1–e26405:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2022:FID

[Nag22] Ágnes Nagy. Fisher information and density functional theory. *International Journal of Quantum Chemistry*, 122(8): e26679:1–e26679:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nath:2022:IAR

[Nat22] Debraj Nath. An introduction to analysis of Rényi complexity ratio of quantum states for central potential. *International Journal of Quantum Chemistry*, 122(1):e26816:1–e26816:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakata:2020:AFS

[NF20] Hiroya Nakata and Dmitri G. Fedorov. Analytic first and second derivatives of the energy in the fragment molecular orbital method combined with molecular mechanics. *International Journal of Quantum Chemistry*, 120(24):e26414:1–

e26414:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nabi:2020:EVM

[NG20] Muskan Nabi and Dinesh C. Gupta. Effect of variation of metal and non-metal elements on various properties of rare-earth-based inverse perovskites Gd_3XY (X = Ga, In and Y = B, N). *International Journal of Quantum Chemistry*, 120 (12):e26197:1–e26197:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakanishi:2020:DSN

[NHNO20] Waro Nakanishi, Satoko Hayashi, Taro Nishide, and Shota Otsuki. Dynamic and static nature of activated interactions in transition states as elucidated by quantum theory of atoms-in-molecules dual functional analysis: a case of ligand exchange at the N of sulfonylimino-λ^3-bromanes. *International Journal of Quantum Chemistry*, 120(4):e26073:1–e26073:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naserian:2021:ISP

[NIA21] Samira Naserian, Mohammad Izadyar, and Foroogh Arkan. Insight into the semiconducting performance of tetraphenyldipyranylidene derivatives in organic field-effect transistors. *International Journal of Quantum Chemistry*, 121(16):qua26678:1–qua26678:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naumov:2021:SET

[NLA+21] Vladimir S. Naumov, Anastasiia S. Loginova, Alexander A. Avdoshin, Stanislav K. Ignatov, Alexey V. Mayorov, Bálint Aradi, and Thomas Frauenheim. Structural, electronic, and thermodynamic properties of TiO_2 /organic clusters: performance of DFTB method with different parameter sets. *International Journal of Quantum Chemistry*, 121(2): e26427:1–e26427:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nath:2021:RVE

[NR21] Debraj Nath and Amlan K. Roy. Ro-vibrational energy and thermodynamic properties of molecules subjected to Deng–Fan potential through an improved approximation. *Inter-*

national Journal of Quantum Chemistry, 121(10):e26616:1–e26616:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nadeem:2022:CCA

[NS22] Muhammad Faisal Nadeem and Ayesha Shabbir. Computing and comparative analysis of topological invariants of Y-junction carbon nanotubes. *International Journal of Quantum Chemistry*, 122(5):e26847:1–e26847:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naray-Szabo:2022:WMC

[NSM22] Gábor Náray-Szabó and Paul G. Mezey. A wavefunction model to chemical bonding. *International Journal of Quantum Chemistry*, 122(8):e26686:1–e26686:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nie:2021:FFR

[NYX+21] Xing Nie, Yong Yang, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. Fatigue and fatigue resistance in S_1 excited state diarylethenes in electric fields. *International Journal of Quantum Chemistry*, 121(6):e26527:1–e26527:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasiri:2020:QMC

[NZ20] Saeed Nasiri and Mansour Zahedi. Quantum Monte Carlo study of ground and first excited state of C, N, O, F, and Ne atoms using Slater–Jastrow-Backflow wave function. *International Journal of Quantum Chemistry*, 120(11):e26187:1–e26187:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasser:2021:CIE

[NZAH21] Ibraheem Nasser, Mostafa Zeama, and Afaf Abdel-Hady. Calculation of information entropies for the $1s^2$ state of helium-like ions. *International Journal of Quantum Chemistry*, 121(5):e26499:1–e26499:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olejniczak:2021:RFD

[OAJ21] Małgorzata Olejniczak, Andrej Antusek, and Michał Jaszuński. Relativistic frozen density embedding calculations of solvent effects on the nuclear magnetic resonance shielding constants of transition metal nuclei. *International Journal of Quantum Chemistry*, 121(22):e26789:1–e26789:??, November 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okun:2021:RC

[OB21a] Pavel Okun and Kieron Burke. Response to comment. *International Journal of Quantum Chemistry*, 121(19):e26767:1–e26767:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okun:2021:UAE

[OB21b] Pavel Okun and Kieron Burke. Uncommonly accurate energies for the general quartic oscillator. *International Journal of Quantum Chemistry*, 121(7):e26554:1–e26554:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [TdV21].

Oner:2021:RCE

[ÖÇÖ21] Alara Öner and Nihan Çelebi-Ölçüm. Rapid computational evaluation of small-molecule hydrolase mimics for preorganized H-bond networks. *International Journal of Quantum Chemistry*, 121(2):e26423:1–e26423:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

On:2022:FPI

[OGSPP^{+}22] Vo Van On, J. Guerrero-Sanchez, R. Ponce-Pérez, J. F. Rivas-Silva, Gregorio H. Cocoletzi, and D. M. Hoat. First-principles investigation of the $(\mathrm{HfSe}_2)_{4-n}$-$(\mathrm{HfSSe})_n$ ($n = 0, 1, 2, 3, 4$) lateral heterostructures. *International Journal of Quantum Chemistry*, 122(6):e26857:1–e26857:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olejniczak:2020:TDA

[OGT20] Małgorzata Olejniczak, André Severo Pereira Gomes, and Julien Tierny. A Topological Data Analysis perspective on noncovalent interactions in relativistic calculations. *International Journal of Quantum Chemistry*, 120(8):e26133:1–e26133:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olendski:2020:RTE

[Ole20] Oleg Olendski. Rényi and Tsallis entropies of the Dirichlet and Neumann one-dimensional quantum wells. *International Journal of Quantum Chemistry*, 120(12):e26220:1–e26220:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olendski:2021:CAI

[Ole21] O. Olendski. Comparative analysis of information measures of the Dirichlet and Neumann two-dimensional quantum dots. *International Journal of Quantum Chemistry*, 121(4): e26455:1–e26455:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ouadah:2021:TQA

[OMA21] Ouahiba Ouadah, Ghouti Merad, and Hayet Si Abdelkader. Theoretic quantum analysis of mechanical and electronic properties of TiAl-M (M = Mo, W, Cu and Zn). *International Journal of Quantum Chemistry*, 121(9):e26590:1–e26590:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

On:2021:PEE

[ONH+21] Vo Van On, Duy Khanh Nguyen, D. M. Hoat, R. Ponce-Pérez, J. F. Rivas-Silva, and Gregorio H. Cocoletzi. Pressure effects on the electronic, magnetic, thermoelectric, and thermodynamic properties of Mn_2CoSi half-metallic compound. *International Journal of Quantum Chemistry*, 121(4):e26445:1–e26445:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onate:2021:FIV

[OO21a] Clement A. Onate and Michael C. Onyeaju. Fisher information of a vector potential for time-dependent Feinberg–Horodecki equation. *International Journal of Quantum Chemistry*, 121(6):e26543:1–e26543:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [NACP21] and reply [OO21b].

Onate:2021:RCF

[OO21b] Clement A. Onate and Michael C. Onyeaju. Reply to the comment on “Fisher information of a vector potential for time-dependent Feinberg–Horodecki”. *International Journal of Quantum Chemistry*, 121(12):e26629:1–e26629:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [OO21a].

Oliveira:2021:LRI

[OR21] João P. C. Oliveira and Roberto Rivelino. Linear response of the indirect J-coupling alternation to the energy gap of increasing π-conjugated oligomers. *International Journal of Quantum Chemistry*, 121(4):e26474:1–e26474:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2020:QMM

[ORL+20a] Marisa C. Oliveira, Renan A. P. Ribeiro, Elson Longo, Mauricio R. D. Bomio, and Sergio R. de Lázaro. Quantum mechanical modeling of Zn-based spinel oxides: Assessing the structural, vibrational, and electronic properties. *International Journal of Quantum Chemistry*, 120(22):e26368:1–e26368:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2020:TDP

[ORL+20b] Marisa C. Oliveira, Renan A. P. Ribeiro, Elson Longo, Maurício R. D. Bomio, Fabiana V. Motta, and Sergio R. de Lazaro. Temperature dependence on phase evolution in the $BaTiO_3$ polytypes studied using ab initio calculations. *International Journal of Quantum Chemistry*, 120 (1):e26054:1–e26054:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2020:FPI

[Pan20] Yong Pan. First-principles investigation of structural, electronic, and optical properties of transition metal-doped C40 $CrSi_2$. *International Journal of Quantum Chemistry*, 120(22):e26401:1–e26401:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2022:NIS

[Pan22] Yong Pan. New insight into the structural, mechanical, electronic, and thermodynamic properties of the monoclinic $TMAl_3$-type aluminides. *International Journal of Quantum Chemistry*, 122(2):e26825:1–e26825:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pachori:2021:MSH

[PAS+21] Sanjay Pachori, Rohit Agarwal, Akash Shukla, Upasana Rani, and Ajay Singh Verma. Mechanically stable with highly absorptive formamidinium lead halide perovskites $[HC(NH_2)_2PbX_3$; X = Br, Cl]: Recent advances and perspectives. *International Journal of Quantum Chemistry*, 121 (15):e26671:1–e26671:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pandey:2021:ISA

[PASS21] Chhama Pandey, Gulzar Ahmed, Ramesh Sharma, and Yamini Sharma. Ab initio study of anisotropic properties in isomorphic TiX_2 (X = S, Se, Te). *International Journal of Quantum Chemistry*, 121(8):e26575:1–e26575:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poddar:2022:LMO

[PC22] Arpita Poddar and Pratim Kumar Chattaraj. Li_4EPc: a metallo-organic electride comprising metal-nitrogen bonds. *International Journal of Quantum Chemistry*, 122(6): e26856:1–e26856:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:2020:NCB

[PCKP20] Fabio E. Penotti, David L. Cooper, Peter B. Karadakov, and Robert Ponec. Nature of the chemical bonding in D_{3h} $[MH_3M]^+$ cations (M = Be, Mg). *International Journal of Quantum Chemistry*, 120(11):e26183:1–e26183:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petrov:2022:PIM

[PD22] Alexander I. Petrov and Ilya D. Dergachev. Platinum(II)-mediated disulfide/thiolate interconversion in organic disulfides: Density functional theory thermodynamic study. *International Journal of Quantum Chemistry*, 122(5): e26849:1–e26849:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peverati:2021:FED

[Pev21] Roberto Peverati. Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. *International Journal of Quantum Chemistry*, 121(1):e26379:1–e26379:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pablo-Garcia:2021:TCI

[PGÁML21] Sergio Pablo-García, Moises Álvarez-Moreno, and Núria López. Turning chemistry into information for heterogeneous catalysis. *International Journal of Quantum Chemistry*, 121(1):e26382:1–e26382:??, January 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paredes-Gil:2020:IRD

[PGPHAPM20] Katherine Paredes-Gil, Dayán Páez-Hernández, Ramiro Arratia-Pérez, and Fernando Mendizábal. Insights into the role of D–A–π–A type pro-aromatic organic dyes with thieno[3,4-b]pyrazine as A acceptor group into dye-sensitized solar-cells. A TD-DFT/periodic DFT study. *International Journal of Quantum Chemistry*, 120(5): e26108:1–e26108:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2020:ABS

[PGROM20] José J. Peña, Jesús García-Ravelo, Gerardo Ovando, and Jesús Morales. Approximate l-bound state solutions of q-deformed exponential-type potentials. *International Journal of Quantum Chemistry*, 120(11):e26189:1–e26189:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pakravesh:2021:MET

[PIA21] Faezeh Pakravesh, Mohammad Izadyar, and Foroogh Arkan. Molecular engineering of triphenylamine-based metal-free organic dyes for dye-sensitized solar cells. *International Journal of Quantum Chemistry*, 121(10):e26620:1–e26620:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2020:IHP

[PJ20a] Yong Pan and Yanlin Jia. The influence of high pressure on the structural stability, Vickers hardness and mechanical properties of Re and Ru dodecaborides. *International Journal of Quantum Chemistry*, 120(6):e26130:1–e26130:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez-Jorda:2020:IEP

[PJ20b] José M. Pérez-Jordá. Inverting the external-potential-to-electron density map in systems of electrons by minimization of a least-squares fit functional for analytic potentials. *International Journal of Quantum Chemistry*, 120(1):e26052:1–e26052:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paudel:2020:HMM

[PKBZ20] Ramesh Paudel, Gopi Chandra Kaphle, Mohammed Batouche, and Jingchuan Zhu. Half-metallicity, magnetism, mechanical, thermal, and phonon properties of FeCrTe and FeCrSe half-Heusler alloys under pressure. *International Journal of Quantum Chemistry*, 120(24):e26417:1–e26417:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2020:IAE

[PL20] Yong Pan and Yuanhua Lin. Influence of alloying elements on the mechanical and thermodynamic properties of ZrB_{12} ceramics from first-principles calculations. *International Journal of Quantum Chemistry*, 120(12):e26217:1–e26217:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Phillips:2020:SEP

[PLT+20] James A. Phillips, Anna R. Ley, Patrick W. Treacy, Benjamin M. Wahl, Brittany C. Zehner, Kelling J. Donald, and Samuel Gillespie. Structural and energetic properties of RMX_3-NH_3 complexes. *International Journal of Quantum Chemistry*, 120(20):e26383:1–e26383:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patra:2020:AHC

[PM20] Shanti G. Patra and Nilangshu Mandal. Aromaticity of *N*-heterocyclic carbene and its analogues: Magnetically induced ring current perspective. *International Journal of Quantum Chemistry*, 120(9):e26152:1–e26152:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pedersen:2022:WEL

[PM22] Jacob Pedersen and Kurt V. Mikkelsen. Working equation of linear response time-dependent density functional theory: First-order polarization propagator approximation. *International Journal of Quantum Chemistry*, 122(11):e26891:1–e26891:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pereira:2021:DSM

[PMdN21] Lucas Carvalho Pereira, Bruno Spolon Marangoni, and Valter Aragão do Nascimento. Dynamics and stability of matter-wave solitons in cigar-shaped Bose–Einstein condensates dragged by Pöschl–Teller potential. *International Journal of Quantum Chemistry*, 121(11):e26634:1–e26634:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2021:ODM

[PMGR+21] José Juan Peña, Jesús Morales, Jesús García-Ravelo, Jaime Avendaño, and Jesús García-Martínez. On the one-dimensional Morse potential as limit of a class of multi-parameter exponential-type radial potential. *International Journal of Quantum Chemistry*, 121(7):e26572:1–e26572:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Punter:2020:PFS

[PNC20] Alexander Punter, Paola Nava, and Yannick Carissan. Pseudopotential-fragment spectroscopy for organic molecules and carbon allotropes. *International Journal of Quantum Chemistry*, 120(11):e26180:1–e26180:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PonsViver:2019:PIL

[Pon19] Miquel Pons Viver. The practical implementation of Löwdin's method for spin projection. *International Journal of Quantum Chemistry*, 119(4):e25770:1–e25770:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Yos20].

Pu:2021:PSM

[PP21] Delin Pu and Yong Pan. Prediction the structure, mechanical properties and melting point of $D8_m$-Mo_5 SiB_2 and Cmcm-Mo_5 SiB_2. *International Journal of Quantum Chemistry*, 121(18):e26751:1–e26751:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pedrajas:2020:BDM

[PPCF+20] Elena Pedrajas, José A. Pino-Chamorro, Montserrat Ferrer, M. Jesús Fernández-Trujillo, Rosa Llusar, Manuel Martínez, Manuel G. Basallote, and Andrés G. Algarra. Benchmarking of DFT methods using experimental free energies and volumes of activation for the cycloaddition of alkynes to cuboidal Mo_3 S_4 clusters. *International Journal of Quantum Chemistry*, 120(19):e26353:1–e26353:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pereira:2021:PVN

[PPR21] Ander Francisco Pereira, Ingrid Guarnetti Prandi, and Teodorico Castro Ramalho. Parameterization and validation of a new force field for Pt(II) complexes of 2-(4'-amino-2'-hydroxyphenyl)benzothiazole. *International Journal of Quantum Chemistry*, 121(6):e26525:1–e26525:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pandya:2022:TSI

[PSJ22] Jalaja B. Pandya, Satyam M. Shinde, and Prafulla K. Jha. Theoretical study on the interaction of flutamide anticancer drug with cucurbit[n]uril ($n = 5$–8) as a drug delivery system. *International Journal of Quantum Chemistry*, 122(12): e26899:1–e26899:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paquier:2021:SRC

[PT21] Julien Paquier and Julien Toulouse. Short-range correlation energy of the relativistic homogeneous electron gas. *International Journal of Quantum Chemistry*, 121(16):e26685:1–e26685:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parsazadeh:2020:DNO

[PVR20] Hasibeh Parsazadeh, Younes Valadbeigi, and Morteza Rouhani. Design of new organic superacids with fused and isolated pyrrole and cyclopentadiene rings and assessment of effect of -BX_2 (X = H, F, Cl, CN) substituents on the acidity enhancement: a DFT analysis. *International Journal of Quantum Chemistry*, 120(8):e26144:1–e26144:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patel:2020:LES

[PZGH+20] Megha Patel, Jiayun Zhong, Konrad S. Gomez-Haibach, Maria A. Gomez, and Graham King. Low-energy $Sr_2MSbO_{5.5}$ (M = Ca and Sr) structures show significant distortions near oxygen vacancies. *International Journal of Quantum Chemistry*, 120(20):e26356:1–e26356:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2022:EBP

[QDC+22] Yongfeng Qu, Jijun Ding, Haixia Chen, Wenbo Hu, and Huiqing Fan. The effect of both Pt decoration and the defects on the adsorption of graphene for SO_2. *International Journal of Quantum Chemistry*, 122(11):e26888:1–e26888:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintal:2021:AIA

[QDOC+21] Alan Quintal, Eugenia Dzib, Filiberto Ortíz-Chi, Pablo Jaque, Albeiro Restrepo, and Gabriel Merino. Automating the IRC-Analysis within Eyringpy. *International Journal of Quantum Chemistry*, 121(16):e26684:1–e26684:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quattrociocchi:2021:MVD

[QdOdMC+21] Daniel G. S. Quattrociocchi, Antonio Rafael de Oliveira, José Walkimar de Mesquita Carneiro, Carlos Murilo Romero Rocha, and António J. C. Varandas. MP2 versus density functional theory calculations in CO_2 -sequestration reactions with anions: Basis set extrapolation and solvent effects. *International Journal of Quantum Chemistry*, 121(8): e26583:1–e26583:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintana:2020:NMI

[QOM+20] Constanza G. Quintana, Fernanda Ocayo, Raul Guajardo Maturana, John J. Hurtado, and Alvaro Muñoz-Castro. Nature of mercury inclusion in intermediate 6-valence electron $[M@Au_8Hg_x\ (PPh_3)_8]^{n+}$ (M = Au, Pd, Pt; x = 0–2) protected gold superatoms: Insights from relativistic density functional theory calculations. *International Journal of Quantum Chemistry*, 120(2):e26068:1–e26068:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raza:2020:BZI

[RA20] Zahid Raza and Akbar Ali. Bounds on the Zagreb indices for molecular (n, m)-graphs. *International Journal of Quantum Chemistry*, 120(18):e26333:1–e26333:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rached:2021:PNQ

[Rac21] Habib Rached. Prediction of a new quaternary Heusler alloy within a good electrical response at high temperature for spintronics applications: DFT calculations. *International Journal of Quantum Chemistry*, 121(12):e26647:1–

e26647:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radenkovic:2021:MAC

[Rad21] Slavko Radenković. A method for analyzing the cyclic electron delocalization interaction between different rings in polycyclic molecules. *International Journal of Quantum Chemistry*, 121(9):e26597:1–e26597:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rani:2021:AIL

[RBJ21] Babita Rani, Vladimir Bubanja, and Vijay K. Jindal. Atomistic insights into lithium adsorption and migration on phosphorus-doped graphene. *International Journal of Quantum Chemistry*, 121(14):e26659:1–e26659:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rossi:2021:CIV

[RBSW21a] Alessandro Rossi, Paul G. Baity, Vera M. Schäfer, and Martin Weides. Cover image, volume 121, issue 14. *International Journal of Quantum Chemistry*, 121(14):e26306:1–e26306:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rossi:2021:QCH

[RBSW21b] Alessandro Rossi, Paul G. Baity, Vera M. Schäfer, and Martin Weides. Quantum computing hardware in the cloud: Should a computational chemist care? *International Journal of Quantum Chemistry*, 121(14):e26688:1–e26688:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rossi:2020:RDU

[RC20] Kevin Rossi and James Cumby. Representations and descriptors unifying the study of molecular and bulk systems. *International Journal of Quantum Chemistry*, 120(8):e26151:1–e26151:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rached:2022:CCI

[RCM+22] Youcef Rached, Messaoud Caid, Mostefa Merabet, Salaheddine Benalia, Habib Rached, Lakhdar Djoudi, Mohamed Mokhtari, and Djamel Rached. A comprehensive computational investigations on the physical properties of TiXSb (X: Ru, Pt) half-Heusler alloys and Ti_2 $RuPtSb_2$ double half-Heusler. *International Journal of Quantum Chemistry*, 122(9):e26875:1–e26875:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2021:ITE

[RDMF21] Nailton Martins Rodrigues, José Diogo Lisboa Dutra, João B. L. Martins, and Ricardo Oliveira Freire. IRMOF-8: Theoretical evaluation of aluminum doping on hydrogen, methane, and hydrogen sulfide adsorption. *International Journal of Quantum Chemistry*, 121(5):e26510:1–e26510:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryzhkov:2021:FPS

[RED21] Mikhail V. Ryzhkov, Andrei N. Enyashin, and Bernard Delley. First-principles study on the plutonium ions interaction with diamide molecules in acid solutions. *International Journal of Quantum Chemistry*, 121(16):e26681:1–e26681:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramanantoanina:2020:TIM

[RG20] Harry Ramanantoanina and Maja Gruden. Theoretical insight into the magnetic circular dichroism of uranium $N_{6,7}$-edge X-ray absorption. *International Journal of Quantum Chemistry*, 120(3):e26081:1–e26081:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2021:ETM

[RHS+21] Yuehong Ren, Qingzhen Han, Qiaozhi Su, Jie Yang, Yuehong Zhao, Hao Wen, and Zhaotan Jiang. Effects of 4d transition metals doping on the photocatalytic activities of anatase TiO_2 (101) surface. *International Journal of Quantum Chemistry*, 121(16):e26683:1–e26683:??, August

15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ranjbakhsh:2020:PDG

[RINHY20] Elnaz Ranjbakhsh, Mohammad Izadyar, Ali Nakhaeipour, and Aziz Habibi-Yangjeh. P-doped g-C_3 N_4 as an efficient photocatalyst for CO_2 conversion into value-added materials: a joint experimental and theoretical study. *International Journal of Quantum Chemistry*, 120(23):e26388:1–e26388:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryzhikov:2021:PES

[RK21] Maxim R. Ryzhikov and Svetlana G. Kozlova. Potential energy surface and band gap landscape of molybdenum and titanium disulfides. *International Journal of Quantum Chemistry*, 121(23):e26803:1–e26803:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rani:2021:ETP

[RKA+21] Upasana Rani, Peeyush Kumar Kamlesh, Rohit Agarwal, Jyoti Kumari, and Ajay Singh Verma. Electronic and thermo-physical properties of double antiperovskites X_6SOA_2 (X = Na, K and A = Cl, Br, I): a non-toxic and efficient energy storage materials. *International Journal of Quantum Chemistry*, 121(19):e26759:1–e26759:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Romanova:2021:IMD

[RKG21] Ksenia Romanova, Alena Kremleva, and Yuriy Galyametdinov. Ab initio molecular dynamics study of the structure and supramolecular organization in mesogenic lanthanum(III) complexes with β-diketones and Lewis bases. *International Journal of Quantum Chemistry*, 121(7): e26569:1–e26569:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ricard:2020:EGT

[RKI20] Timothy C. Ricard, Anup Kumar, and Srinivasan S. Iyengar. Embedded, graph-theoretically defined many-body approximations for wavefunction-in-DFT and DFT-in-DFT:

Applications to gas- and condensed-phase ab initio molecular dynamics, and potential surfaces for quantum nuclear effects. *International Journal of Quantum Chemistry*, 120(21):e26244:1–e26244:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raza:2020:FPI

[RMeH+20] Hafiz Hamid Raza, G. Murtaza, Umm e Hani, Nawaz Muhammad, and Shahid M. Ramay. First-principle investigation of $XSrH_3$ (X = K and Rb) perovskite-type hydrides for hydrogen storage. *International Journal of Quantum Chemistry*, 120(24):e26419:1–e26419:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Montes:2020:LTF

[RMLPGHP20] Luz Ramírez-Montes, William López-Pérez, Rafael González-Hernández, and Carlos Pinilla. Large thermoelectric figure of merit in hexagonal phase of 2D selenium and tellurium. *International Journal of Quantum Chemistry*, 120(17):e26267:1–e26267:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rabeya:2022:SDG

[RMM+22] Ramisha Rabeya, Savisha Mahalingam, Abreeza Manap, Meenaloshini Satgunam, Md. Akhtaruzzaman, and Chin Hua Chia. Structural defects in graphene quantum dots: a review. *International Journal of Quantum Chemistry*, 122(12):e26900:1–e26900:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Redzepovic:2020:SDD

[RMWF20] Izudin Redzepović, Yaping Mao, Zhao Wang, and Boris Furtula. Steiner degree distance indices: Chemical applicability and bounds. *International Journal of Quantum Chemistry*, 120(12):e26209:1–e26209:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rauf:2022:QSPa

[RNA22] Abdul Rauf, Muhammad Naeem, and Adnan Aslam. Quantitative structure-property relationship of edge weighted and degree-based entropy of benzene derivatives. *International Journal of Quantum Chemistry*, 122(3):e26839:1–e26839:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rauf:2022:QSPb

[RNB22] Abdul Rauf, Muhammad Naeem, and Saira Usman Bukhari. Quantitative structure-property relationship of Ev-degree and Ve-degree based topological indices : physico-chemical properties of benzene derivatives. *International Journal of Quantum Chemistry*, 122(5):e26851:1–e26851:??, March 05, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robles-Navarro:2020:ESF

[RNFMC20] Andrés Robles-Navarro, Patricio Fuentealba, Francisco Muñoz, and Carlos Cárdenas. Electronic structure of first and second row atoms under harmonic confinement. *International Journal of Quantum Chemistry*, 120(7):e26132:1–e26132:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robles-Navarro:2021:CNB

[RNRBFC21] Andrés Robles-Navarro, Mariano Rodriguez-Bautista, Patricio Fuentealba, and Carlos Cárdenas. The change in the nature of bonding in the Li_2 dimer under confinement. *International Journal of Quantum Chemistry*, 121(12):e26644:1–e26644:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rohr:2021:NTM

[Röh21] Merle I. S. Röhr. New theoretical methods for the exploration of functional landscapes. *International Journal of Quantum Chemistry*, 121(24):e26747:1–e26747:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2020:TIA

[Roy20] Lisa Roy. Theoretical investigation of an acid catalyst for viable release of H_2 from BN nanotubes: a local pair natural orbital coupled cluster approach. *International Journal of Quantum Chemistry*, 120(15):e26257:1–e26257:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raghunathan:2022:MRM

[RP22] Shampa Raghunathan and U. Deva Priyakumar. Molecular representations for machine learning applications in chemistry. *International Journal of Quantum Chemistry*, 122(7): e26870:1–e26870:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radhakrishnan:2022:MSC

[RPAA22] M. Radhakrishnan, Savari Prabhu, Micheal Arockiaraj, and M. Arulperumjothi. Molecular structural characterization of superphenalene and supertriphenylene. *International Journal of Quantum Chemistry*, 122(2):e26818:1–e26818:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reinhardt:2021:MAP

[RPT21a] Peter Reinhardt, Ilya Popov, and Andrei L. Tchougréeff. Minimum atomic parameter basis sets for elements 1-54 in a Hartree–Fock setting. *International Journal of Quantum Chemistry*, 121(16):e26687:1–e26687:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reinhardt:2021:SDA

[RPT21b] Peter Reinhardt, Ilya Popov, and Andrei L. Tchougréeff. Spatial distribution of atomic electronic density for elements 1–54 as coming from a Hartree–Fock treatment within the minimum atomic parameters paradigm. *International Journal of Quantum Chemistry*, 121(17):e26690:1–e26690:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2021:NBR

[RR21] Gabriel L. Silva Rodrigues and Willian R. Rocha. Nature of the bond, reduction potential, and solvation properties of ruthenium nitrosyl complexes of the type trans-$[Ru(NH_3)_4\ (L)(NO)]^{2+/3+}$ and $[Ru(salen)(L)(NO)]^{2+/3+}$ in different charge and spin states. *International Journal of Quantum Chemistry*, 121(4):e26476:1–e26476:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radenkovic:2022:RVE

[RRD+22] Slavko Radenković, Izudin Redzepović, Sladana Dordević, Boris Furtula, Niko Tratnik, and Petra Zigert Pletersek. Relating vibrational energy with Kekulé- and Clar-structure-based parameters. *International Journal of Quantum Chemistry*, 122(7):e26867:1–e26867:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rada:2021:GPC

[RRS21] Juan Rada, José M. Rodríguez, and José M. Sigarreta. Geometric properties of chemical graphs. *International Journal of Quantum Chemistry*, 121(23):e26798:1–e26798:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rohloff:2022:CNM

[RRSF22] Erik Rohloff, Dominik A. Rudolph, Onno Strolka, and Irmgard Frank. Classical nuclear motion: Does it fail to explain reactions and spectra in certain cases? *International Journal of Quantum Chemistry*, 122(12):e26902:1–e26902:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rahimi:2021:LDA

[RS21] Rezvan Rahimi and Mohammad Solimannejad. Li-decorated Al_2 C monolayer as a potential template for hydrogen storage: a first-principles perspective. *International Journal of Quantum Chemistry*, 121(6):e26528:1–e26528:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rastegar-Sedehi:2020:MEA

[RSBK20] Hamid-Reza Rastegar-Sedehi, Tim Byrnes, and Reza Khordad. Moment expansion approach to the time dynamics of genetic evolution. *International Journal of Quantum Chemistry*, 120(3):e26089:1–e26089:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ray:2021:ASD

[RSD21] Koustuv Ray, Aditya Shankar Sandupatla, and Goutam Deo. Activity and stability descriptors of Ni based alloy catalysts for dry reforming of methane: a density functional theory study. *International Journal of Quantum Chemistry*, 121(8):e26580:1–e26580:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruiz:2022:HPH

[Rui22] María Belén Ruiz. Half-projected Hartree–Fock method: History and application to excited states of the same symmetry as the ground state. *International Journal of Quantum Chemistry*, 122(8):e26889:1–e26889:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2020:CIT

[RYC+20] Hai Chao Ren, Jiao Nan Yuan, Tu Nan Chen, Gurudeeban Selvaraj, Satyavani Kaliamurthi, Xiu Qing Zhang, Dong-Qing Wei, Guang Fu Ji, and Zeng Ming Zhang. Computational insights of two-dimensional infrared spectroscopy under electric fields in phosphorylcholine. *International Journal of Quantum Chemistry*, 120(13):e26169:1–e26169:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sumner:2020:ETM

[SA20] Isaiah Sumner and Hannah Anthony. Electron trajectories in molecular orbitals. *International Journal of Quantum Chemistry*, 120(20):e26371:1–e26371:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahni:2021:SPT

[Sah21] Viraht Sahni. Schrödinger–Pauli theory of electrons: New perspectives. *International Journal of Quantum Chemistry*, 121(7):e26556:1–e26556:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saxena:2021:IDG

[SASA21] Raghav Saxena, V B K Sai Phani Kumar Avanigadda, Raghvendra Singh, and Vishal Agarwal. Ab initio dynamics of gas-phase and aqueous-phase hydrolysis of adenosine triphosphate. *International Journal of Quantum Chemistry*, 121(10):e26615:1–e26615:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2021:ESC

[SBA21] Jayanta K. Saha, Sukhamoy Bhattacharyya, and Sk. Faruque Ahmed. Electronic structure calculations of compressed Li atom using composite technique under Ritz variational framework. *International Journal of Quantum Chemistry*, 121(7):e26570:1–e26570:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2021:MFR

[SBG21] Mateus Xavier Silva, Jadson Cláudio Belchior, and Breno Rodrigues Lamaghere Galvão. Mechanisms for N_3 formation in radiated solid nitrogen: Computational predictions including excited electronic states. *International Journal of Quantum Chemistry*, 121(7):e26562:1–e26562:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2020:DFT

[SBJ20] Ram Singh, Prakash Biswas, and Prateek K. Jha. Density functional theory investigation of structure, stability, and glycerol/hydrogen adsorption on Cu, Cu–Zn, and Cu–ZnO clusters. *International Journal of Quantum Chemistry*, 120 (14):e26239:1–e26239:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sattarova:2022:QCA

[SBM22] Alina F. Sattarova, Yulia N. Biglova, and Akhat G. Mustafin. Quantum-chemical approaches in the study of fullerene and its derivatives by the example of the most typical cycloaddition reactions: a review. *International Journal of Quantum Chemistry*, 122(7):e26863:1–e26863:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simoes:2021:CSS

[SC21] Luís H. Simões and Rodrigo A. Cormanich. Challenges in studying steric interactions in highly strained perhalogenated alkanes and silanes. *International Journal of Quantum Chemistry*, 121(21):e26785:1–e26785:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanhueza:2020:EAH

[SCAD+20] Luis Sanhueza, Diego Cortés-Arriagada, Ramiro Díaz, Paulina Dreyse, Camilo García, Iván A. Gonzalez, and Bárbara Loeb. Effect on the aromaticity of heterocyclic ligands by coordination with ruthenium electron-withdrawing metal centers. *International Journal of Quantum Chemistry*, 120(24):e26412:1–e26412:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sirin:2021:CID

[SCU21] Pinar Seyitdanlioglu Sirin, Pervin Ünal Civcir, and Canan Unaleroglu. A computational insight on designing low electronic energy gap benzothiadiazole/benzoselenadiazole-pyrrole copolymers. *International Journal of Quantum Chemistry*, 121(8):e26585:1–e26585:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sang:2021:TIA

[SCZ21] Shenglong Sang, Fei Chen, and Cong Zhang. Theoretical investigation of aromaticity and charge transfer in emission process of triarylmethyl radicals as OLED materials. *International Journal of Quantum Chemistry*, 121(6):e26522:1–e26522:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solaimani:2020:QIE

[SD20] M. Solaimani and Shi-Hai Dong. Quantum information entropies of multiple quantum well systems in fractional Schrödinger equations. *International Journal of Quantum Chemistry*, 120(5):e26113:1–e26113:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shorifuddoza:2021:ADC

[SDK+21] M. Shorifuddoza, Pretam K. Das, Raihan Kabir, A. K. Fazlul Haque, and M. Alfaz Uddin. Angular distributions and critical minima in the elastic scattering of electrons by atomic copper. *International Journal of Quantum Chemistry*, 121(4):e26460:1–e26460:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2022:TSD

[SDL+22] Chengkuan Shi, Wenjing Dong, Fang Li, Wei Xue, and Yanji Wang. Theoretical study of decomposition of formic acid over Pd catalyst anchored on N-doped graphene. *International Journal of Quantum Chemistry*, 122(13):e26908:1–e26908:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadhukhan:2019:CSQ

[SDS19] Anjan Sadhukhan, Sayantan Dutta, and Jayanta K. Saha. Critical stability and quantum phase transition of screened two-electron system. *International Journal of Quantum Chemistry*, 119(24):e26042:1–e26042:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See corrigendum [SDS20].

Sadhukhan:2020:CCS

[SDS20] Anjan Sadhukhan, Sayantan Dutta, and Jayanta K. Saha. Corrigendum: Critical stability and quantum phase transition of screened two-electron system. *International Journal of Quantum Chemistry*, 120(3):e26084:1–e26084:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [SDS19].

Slavova:2020:SCM

[SE20] Sofia Slavova and Venelin Enchev. Self-catalytic mechanism of prebiotic reactions: From formamide to purine bases. *International Journal of Quantum Chemistry*, 120(19): e26362:1–e26362:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senjean:2020:CED

[SF20a] Bruno Senjean and Emmanuel Fromager. N-centered ensemble density-functional theory for open systems. *International Journal of Quantum Chemistry*, 120(21):e26190:1–e26190:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shields:2020:MHD

[SF20b] George C. Shields and Scott E. Feller. Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances. *International Journal of Quantum Chemistry*, 120(20):e26370:1–e26370:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shalin:2020:EDF

[SFB20] Nikita I. Shalin, Olga D. Fominykh, and Marina Yu. Balakina. Effect of dimer formation via hydrogen bonding on static and dynamic nonlinear optical characteristics of chromophores. *International Journal of Quantum Chemistry*, 120(1):e26061:1–e26061:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santoyo-Flores:2022:TSH

[SFPH22] Juan Julián Santoyo-Flores and Dayán Páez-Hernández. Theoretical study of 8-hydroxyquinoline derivatives as potential antennas in lanthanide complexes: Photophysical properties and elucidation of energy transfer pathways. *International Journal of Quantum Chemistry*, 122(10):e26880:1–e26880:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santana:2021:CIV

[SFT+21a] Adriano Santana, Andreia S. F. Farinha, Aniela Zarzar Toraño, Mahmoud Ibrahim, and Himanshu Mishra. Cover image, volume 121, issue 5. *International Journal of Quantum Chemistry*, 121(5):e26288:1–e26288:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santana:2021:FPA

[SFT+21b] Adriano Santana, Andreia S. F. Farinha, Aniela Zarzar Toraño, Mahmoud Ibrahim, and Himanshu Mishra. A first-principles approach for treating wastewaters. *International Journal of Quantum Chemistry*, 121(5):e26501:1–e26501:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sofi:2020:ISE

[SG20] Shakeel Ahmad Sofi and Dinesh C. Gupta. Investigation of structural, elastic, thermophysical, magneto-electronic, and transport properties of newly tailored Mn-based Heuslers: a density functional theory study. *International Journal of*

Quantum Chemistry, 120(12):e26216:1–e26216:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sofi:2021:RFP

[SG21] Shakeel Ahmad Sofi and Dinesh C. Gupta. Robustness in ferromagnetic phase stability, half-metallic behavior and transport properties of cobalt-based full-Heuslers compounds: a first principles approach. *International Journal of Quantum Chemistry*, 121(6):e26538:1–e26538:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shaw:2020:CPG

[Sha20] Robert A. Shaw. The completeness properties of Gaussian-type orbitals in quantum chemistry. *International Journal of Quantum Chemistry*, 120(17):e26264:1–e26264:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shields:2020:TYE

[Shi20] George C. Shields. Twenty years of exceptional success: the molecular education and research consortium in undergraduate computational chemistry (MERCURY). *International Journal of Quantum Chemistry*, 120(20):e26274:1–e26274:??, October 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shin:2021:DFT

[Shi21] Joong-Won Shin. Density functional theory computational study of $[\mathrm{MoPro\text{-}H}]^{+}$ (M = Pb, Ba, or Pt) complexes in the gas phase. *International Journal of Quantum Chemistry*, 121(6):e26532:1–e26532:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senami:2020:IHB

[SI20] Masato Senami and Keito Ito. Identification of hydrogen bonds using quantum electrodynamics. *International Journal of Quantum Chemistry*, 120(14):e26237:1–e26237:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabagh:2020:PPF

[SIA20] Samira Sabagh, Mohammad Izadyar, and Foroogh Arkan. Photovoltaic properties of the flavonoid-based photosensitizers: Molecular-scale perspective on the natural dye solar cells. *International Journal of Quantum Chemistry*, 120(10): e26171:1–e26171:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabagh:2021:IIP

[SIA21] Samira Sabagh, Mohammad Izadyar, and Foroogh Arkan. Insight into incident photon to current conversion efficiency in chlorophylls. *International Journal of Quantum Chemistry*, 121(5):e26483:1–e26483:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2020:SEP

[SJ20] Subhasish Saha and Jobin Jose. Shannon entropy as a predictor of avoided crossing in confined atoms. *International Journal of Quantum Chemistry*, 120(22):e26374:1–e26374:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarkar:2020:HBI

[SK20] Ranjini Sarkar and Tarun Kumar Kundu. Hydrogen bond interactions of hydrated aluminum nitrate with PVDF, PVDF-TrFE, and PVDF-HFP: a density functional theory-based illustration. *International Journal of Quantum Chemistry*, 120(17):e26328:1–e26328:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Semenov:2021:BDF

[SK21] Valentin A. Semenov and Leonid B. Krivdin. Benchmark density functional theory calculations of ^{13}C NMR chemical shifts of the natural antimalarial compounds with a new basis set 3z-S. *International Journal of Quantum Chemistry*, 121(12):e26639:1–e26639:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Steinmetzer:2021:PEP

[SKG21] Johannes Steinmetzer, Stephan Kupfer, and Stefanie Gräfe. pysisyphus: Exploring potential energy surfaces in ground and excited states. *International Journal of Quantum Chemistry*, 121(3):e26390:1–e26390:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shubin:2021:FOO

[SKR+21] Aleksandr A. Shubin, Viktor Yu. Kovalskii, Sergey Ph. Ruzankin, Igor L. Zilberberg, Valentin N. Parmon, Felix N. Tomilin, and Pavel V. Avramov. The $Fe^{IV}O\cdot$ oxyl unit as a key intermediate in water oxidation on the Fe^{III}–hydroxide: DFT predictions. *International Journal of Quantum Chemistry*, 121(10):e26610:1–e26610:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutton:2020:SCK

[SLdS20] Catherine C. R. Sutton, Chia-Yang Lim, and Gabriel da Silva. Self-catalyzed keto-enol tautomerization of malonic acid. *International Journal of Quantum Chemistry*, 120 (5):e26114:1–e26114:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2022:TDE

[sLhZX+22] Ru song Li, Xiao hua Zhou, Zheng Xie, Ling yun Kong, Deng wu Wang, and Yang Wang. Temperature-dependent electronic properties for $4f$ states in cerium mononitride. *International Journal of Quantum Chemistry*, 122(11): e26896:1–e26896:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2020:MOV

[sLLqX+20] Ru song Li, Xing Lu, Du qiang Xin, Jin tao Wang, and Bing yun Ao. Magnetic order and valence fluctuation in a Pu–Ga intermetallic compound studied via a first principles calculation. *International Journal of Quantum Chemistry*, 120(4): e26105:1–e26105:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salazar:2020:SIE

[SLPS20] Saúl J. C. Salazar, Humberto G. Laguna, Vinod Prasad, and Robin P. Sagar. Shannon-information entropy sum in the confined hydrogenic atom. *International Journal of Quantum Chemistry*, 120(11):e26188:1–e26188:??, June 5, 2020.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salvador:2022:BSS

[SM22] Pedro Salvador and István Mayer. A basis set superposition error-free second-order perturbation theory from Hermitian chemical Hamiltonian approach self-consistent field canonic orbitals. *International Journal of Quantum Chemistry*, 122 (8):e26777:1–e26777:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schmitt-Monreal:2020:FDE

[SMJ20] Daniel Schmitt-Monreal and Christoph R. Jacob. Frozen-density embedding-based many-body expansions. *International Journal of Quantum Chemistry*, 120(21):e26228:1–e26228:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sullivan:2021:SCI

[SN21] Mason Sullivan and Fedor Y. Naumkin. Supramolecular complexes with insertion-enhanced polarity and tuned IR spectra. *International Journal of Quantum Chemistry*, 121 (6):e26534:1–e26534:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sorensen:2021:NTN

[Sør21] Lasse K. Sørensen. Nakatsuji's theorem of the necessary and sufficient conditions of the wave function revisited. *International Journal of Quantum Chemistry*, 121(23):e26805:1–e26805:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sebastianelli:2020:FMO

[SP20a] Paolo Sebastianelli and Rodolfo G. Pereyra. Frontier molecular orbital analysis for determining the equilibrium geometries of atmospheric prenucleation complexes. *International Journal of Quantum Chemistry*, 120(3):e26060:1–e26060:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stemmle:2020:ECE

[SP20b] Christian Stemmle and Beate Paulus. Electron correlation effects in cobalt fluorides CoF_n. *International Journal of*

Quantum Chemistry, 120(12):e26203:1–e26203:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sangolkar:2022:DFT

[SPF+22] Akanksha Ashok Sangolkar, Pooja, Mohmmad Faizan, Rubi Agrawal, and Ravinder Pawar. Density functional theory study of graphene adhesion on WX_2 (X = S and Se) monolayer: Role of atom vacancy and atomic reorganization defects. *International Journal of Quantum Chemistry*, 122(9): e26871:1–e26871:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sims:2021:ECH

[SPR21] James S. Sims, Bholanath Padhy, and María Belén Ruiz. Exponentially correlated Hylleraas-configuration interaction nonrelativistic energy of the ^{1}S ground state of the helium atom. *International Journal of Quantum Chemistry*, 121(4): e26470:1–e26470:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sims:2022:ECH

[SPR22] James S. Sims, Bholanath Padhy, and María Belén Ruiz. Exponentially correlated Hylleraas-configuration interaction studies of atomic systems. II. Non-relativistic energies of the 1 ^{1}S through 6 ^{1}S states of the Li^+ ion. *International Journal of Quantum Chemistry*, 122(1):e26823:1–e26823:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sharma:2020:SHP

[SRH20] Rajesh O. Sharma, Tapio T. Rantala, and Philip E. Hoggan. Selective hydrogen production at Pt(111) investigated by Quantum Monte Carlo methods for metal catalysis. *International Journal of Quantum Chemistry*, 120(11):e26198:1–e26198:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Subramani:2021:KDM

[SRS21] Mohanapriya Subramani, Akilan Rajamani, and Ramasamy Shankar. Kinetics and degradation mechanism of atmospheric isoprene (2-methyl-1, 3-butadiene (C_5H_8)) with chlorine radical and its derivatives — a theoretical study.

International Journal of Quantum Chemistry, 121(7): e26573:1–e26573:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sharma:2021:NSS

[SS21] Aditi Sharma and Oruganti S. K. S. Sastri. Numerical solution of Schrodinger equation for rotating Morse potential using matrix methods with Fourier sine basis and optimization using variational Monte-Carlo approach. *International Journal of Quantum Chemistry*, 121(16):e26682:1–e26682:??, August 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sobrino:2022:ANC

[SSD22] Nahual Sobrino and Jesus S.-Dehesa. Algebraic L_q norms and complexity-like properties of Jacobi polynomials: Degree and parameter asymptotics. *International Journal of Quantum Chemistry*, 122(6):e26858:1–e26858:??, March 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabet-Sarvestani:2021:SEM

[SSEI21] Hossein Sabet-Sarvestani, Hossein Eshghi, and Mohammad Izadyar. Substituent effects and mechanism studies in CO_2 transformation to benzoxazinone derivatives as worthwhile N-containing heterocycles: Insight from Density functional theory. *International Journal of Quantum Chemistry*, 121(21):e26784:1–e26784:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabet-Sarvestani:2020:MEP

[SSIE20] Hossein Sabet-Sarvestani, Mohammad Izadyar, and Hossein Eshghi. Molecular electrostatic potential at nuclear position as a new concept in evaluation of the substitution effects of intramolecular B/N frustrated Lewis pairs in H_2 splitting and CO_2 reduction. *International Journal of Quantum Chemistry*, 120(24):e26416:1–e26416:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabet-Sarvestani:2021:TDU

[SSIE21] Hossein Sabet-Sarvestani, Mohammad Izadyar, and Hossein Eshghi. Theoretical designing and understanding of the performances of B–H bridged organocatalysts by π-conjugated molecules in CO_2 hydroboration. *International Journal of Quantum Chemistry*, 121(5):e26512:1–e26512:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Semenov:2020:NSS

[SSK20] Valentin A. Semenov, Dmitry O. Samultsev, and Leonid B. Krivdin. ^{1}H and ^{13}C NMR spectra of Strychnos alkaloids: Selected NMR updates. *International Journal of Quantum Chemistry*, 120(19):e26348:1–e26348:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surjan:2022:EMI

[SSL22] Péter R. Surján, Ágnes Szabados, and György Lendvay. Editorial: In memoriam István Mayer. *International Journal of Quantum Chemistry*, 122(8):e26885:1–e26885:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stauch:2021:QCM

[Sta21] Tim Stauch. Quantum chemical modeling of molecules under pressure. *International Journal of Quantum Chemistry*, 121(3):e26208:1–e26208:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suleiman:2021:GIB

[STF21] Motasem Suleiman, Fioralba Taullaj, and Ulrich Fekl. Group-IV-based selective C–H bond activation of a diamondoid — a density functional theory study. *International Journal of Quantum Chemistry*, 121(11):e26638:1–e26638:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sakagami:2020:HDA

[STI20] Hiroki Sakagami, Masanori Tachikawa, and Takayoshi Ishimoto. Hydrogen/ deuterium adsorption and absorption properties on and in palladium using a combined plane wave and localized basis set method. *International Journal of Quantum Chemistry*, 120(16):e26275:1–e26275:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scholz:2020:AER

[STN20] Linus Scholz, Johannes Tölle, and Johannes Neugebauer. Analysis of environment response effects on excitation energies within subsystem-based time-dependent density-functional theory. *International Journal of Quantum Chemistry*, 120(21):e26213:1–e26213:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugiura:2020:TCP

[STT20] Yutaro Sugiura, Toshiyuki Takayanagi, and Masanori Tachikawa. Theoretical calculation of positron annihilation spectrum using positron-electron correlation-polarization potential. *International Journal of Quantum Chemistry*, 120(22):e26376:1–e26376:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shunaev:2020:IFS

[SUG20] Vladislav V. Shunaev, Arseni V. Ushakov, and Olga E. Glukhova. Increase of γ-Fe_2O_3 /CNT composite quantum capacitance by structural design for performance optimization of electrode materials. *International Journal of Quantum Chemistry*, 120(9):e26165:1–e26165:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surjan:2020:IFQ

[Sur20] Péter R. Surján. Introducing the γ function in quantum theory. *International Journal of Quantum Chemistry*, 120 (13):e26221:1–e26221:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Sur22].

Surjan:2022:EIF

[Sur22] Péter R. Surján. Erratum to: Introducing the γ function in quantum theory, Int. J. Quantum. Chem. **120** e26221 (2020). *International Journal of Quantum Chemistry*, 122 (7):e26869:1–e26869:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Sur20].

S:2021:FDI

[SV21] Lekshmi R. S. and Sivaranjana Reddy Vennapusa. Formation and decay of intersystem crossing receiver triplet state in terthiophene and quaterthiophene. *International Journal of Quantum Chemistry*, 121(15):e26677:1–e26677:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sumita:2021:ALM

[SY21] Masato Sumita and Naruki Yoshikawa. Augmented Lagrangian method for spin-coupled wave function. *International Journal of Quantum Chemistry*, 121(18):e26746:1–e26746:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2021:TIL

[SYL+21] Hao Sun, Xiu Yin, Zhi-Peng Liu, Shu-Li Wei, Jian-Zhong Fan, Li-Li Lin, and Yu-Ping Sun. Theoretical insights on the luminescent mechanism of an efficient aggregation-induced nondoped delayed fluorescence emitter using QM/MM method. *International Journal of Quantum Chemistry*, 121(5):e26490:1–e26490:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2021:TSA

[SYT+21] Yanan Sun, Junfang Yao, Yizhen Tang, Yunju Zhang, Wenzhong Wu, and Jingyu Sun. Theoretical study on the atmospheric degradation mechanism and subsequent products of E,E-2,4-hexadienal with hydroxyl radical. *International Journal of Quantum Chemistry*, 121(7):e26563:1–e26563:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shaker:2022:GDM

[SZMM22] Hani Shaker, Mian Muhammad Zobair, Hafiz Muhammad Asif Mehmood, and Mehar Ali Malik. Gourava descriptors of multi-dimensional flat and stable tri-hexagonal boron nanotubes. *International Journal of Quantum Chemistry*, 122(2):e26829:1–e26829:??, January 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thompson:2021:ITW

[TAS21] David C. Thompson, James S. M. Anderson, and K. D. Sen. Information theory and Wigner crystallization: a model perspective. *International Journal of Quantum Chemistry*, 121 (7):e26549:1–e26549:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tao:2021:ERB

[TCL+21] Neng Tao, Yuan Cheng, Song Lu, Haoran Xing, Muhammad Usman Shahid, Siuming Lo, and Heping Zhang. Experimental and ReaxFF-based molecular dynamics studies of the reaction of oxygen with DR-2 as a low global warming potential working fluid. *International Journal of Quantum Chemistry*, 121(23):e26806:1–e26806:??, December 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tirri:2020:CCN

[TCSG+20] Bernardino Tirri, Ilaria Ciofini, Juan C. Sancho-García, Carlo Adamo, and Éric Brémond. Computation of covalent and noncovalent structural parameters at low computational cost: Efficiency of the DH-SVPD method. *International Journal of Quantum Chemistry*, 120(13):e26233:1–e26233:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tao:2022:TDF

[TCX+22] Neng Tao, Yuan Cheng, Haoran Xing, Siuming Lo, Song Lu, and Heping Zhang. Thermal decomposition and fire-extinguishing mechanism of $N(CF_2CF_3)_3$ by ReaxFF-based molecular dynamics simulation and density functional theory calculation. *International Journal of Quantum Chemistry*, 122(12):e26898:1–e26898:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Turbiner:2021:CUA

[TdV21] Alexander V. Turbiner and Juan Carlos del Valle. Comment on: Uncommonly accurate energies for the general quartic oscillator. *International Journal of Quantum Chemistry*, 121(19):e26766:1–e26766:??, October 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [OB21b].

Tang:2021:ABA

[THL+21] Yingqi Tang, Wenbo Huai, Hao Li, Xiaotong Mao, Ju Xie, Jin Yong Lee, and Aiping Fu. Adsorption of $[BF_4]^-$ anion-based ionic liquids on phosphorene, arsenene, and antimonene: a density functional theory study. *International Journal of Quantum Chemistry*, 121(15):e26668:1–e26668:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tavakol:2020:UOC

[THS20] Hossein Tavakol, Fahimeh Hassani, and Dana Shahabi. Using ONIOM calculations to investigate the abilities of simple and nitrogen, boron, sulfur-doped carbon nanotubes in sensing of carbon monoxide. *International Journal of Quantum Chemistry*, 120(12):e26214:1–e26214:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2021:TRT

[Tia21] Wen-Juan Tian. Triple-ring tubular MB_{36} (M = Mg, Ca, Sr, Ba) with threefold aromaticity. *International Journal of Quantum Chemistry*, 121(9):e26595:1–e26595:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Temen:2020:HEM

[TJA20] Story Temen, Amber Jain, and Alexey V. Akimov. Hierarchical equations of motion in the Libra software package. *International Journal of Quantum Chemistry*, 120(22): e26373:1–e26373:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tariq:2021:TEM

[TMH21] Saad Tariq, Ahmad A. Mubarak, and Farida Hamioud. Tuning the electronic and magnetic properties of $CoZr_xNb_{1-x}FeSi$ alloys for spintronic and thermoelectric applications. *International Journal of Quantum Chemistry*, 121(12):e26628:1–e26628:??, June 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tao:2020:CSA

[TPB+20] Yunwen Tao, Zheng Pei, Nicole Bellonzi, Yuezhi Mao, Zhu Zou, Wanzhen Liang, Zhibo Yang, and Yihan Shao. Constructing spin-adiabatic states for the modeling of spin-crossing reactions. I. A shared-orbital implementation. *International Journal of Quantum Chemistry*, 120 (6):e26123:1–e26123:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toranzo:2020:ASI

[TPCSD20] Irene V. Toranzo, David Puertas-Centeno, Nahual Sobrino, and Jesús S. Dehesa. Analytical Shannon information entropies for all discrete multidimensional hydrogenic states. *International Journal of Quantum Chemistry*, 120(2):e26077:1–e26077:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tzeli:2020:SES

[TPT20] Demeter Tzeli, Ioannis D. Petsalakis, and Giannoula Theodorakopoulos. The solvent effect on a styryl-bodipy derivative functioning as an AND molecular logic gate. *International Journal of Quantum Chemistry*, 120(11): e26181:1–e26181:??, June 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Treto-Suarez:2020:RDC

[TSHRS+20] Manuel A. Treto-Suárez, Yoan Hidalgo-Rosa, Eduardo Schott, Ximena Zarate, and Dayan Páez-Hernández. Radiative decay channel assessment to understand the sensing mechanism of a fluorescent turn-on Al^{3+} chemosensor. *International Journal of Quantum Chemistry*, 120(3): e26083:1–e26083:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talukder:2021:TSM

[TSN+21] Srijeeta Talukder, Dipayan Seal, Pulak Naskar, Pinaki Chaudhury, and Subhasree Ghosh. A two state model study of photo-detachment dynamics driven by an optimally designed polychromatic field: a simulated annealing based optimisation. *International Journal of Quantum Chemistry*, 121(15):e26676:1–e26676:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teng:2020:TSN

[TSW+20] Yunyang Teng, Qi Sheng, Hui Weng, Zhongjun Zhou, Xuri Huang, Zhiru Li, and Tao Zhang. Theoretical study of a novel organic electride with large nonlinear optical responses. *International Journal of Quantum Chemistry*, 120 (14):e26235:1–e26235:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thirumoorthy:2021:FCE

[TT21a] Krishnan Thirumoorthy and Venkatesan S. Thimmakondu. Flat crown ethers with planar tetracoordinate carbon atoms. *International Journal of Quantum Chemistry*, 121 (5):e26479:1–e26479:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tran:2021:DMR

[TT21b] Van Tan Tran and Quoc Tri Tran. A density matrix renormalization group investigation on the electronic states of $\mathrm{MnGe}_n^{-/0/+}$ (n = 1–3) clusters. *International Journal of Quantum Chemistry*, 121(10):e26619:1–e26619:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsai:2020:NDB

[TTTH20] Cheng-Cheng Tsai, Zhi-Yao Tsai, Ming-Yu Tseng, and Wei-Ping Hu. A new database and benchmark of the bond energies of noble-gas-containing molecules. *International Journal of Quantum Chemistry*, 120(14):e26238:1–e26238:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Turbiner:2021:UCA

[TVdVN21] Alexander V. Turbiner, Juan Carlos Lopez Vieyra, Juan Carlos del Valle, and Daniel Julia Nader. Ultra-compact accurate wave functions for He-like and Li-like iso-electronic sequences and variational calculus: I. Ground state. *International Journal of Quantum Chemistry*, 121(8):e26586:1–e26586:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Turbiner:2022:UCA

[TVdVN22] Alexander V. Turbiner, Juan Carlos Lopez Vieyra, Juan Carlos del Valle, and Daniel Julian Nader. Ultra-compact accurate wave functions for He-like and Li-like iso-electronic sequences and variational calculus: II. Spin-singlet (excited) and spin-triplet (lowest) states of helium sequence. *International Journal of Quantum Chemistry*, 122(9):e26879:1–e26879:??, May 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2021:CLE

[TWT+21] Jia-Min Tang, Yin-Feng Wang, Qin Tian, Xue-Xia Liu, Zhi-jun Wang, Jiangen Huang, Hua-Rong Zhang, Kai Yang, and Zhi-Ru Li. Conversions of localized excess electrons and spin states under external electric field: Inter-cage electron-transfer isomer $(C_{20}F_{20})_3$ &K_2. *International Journal of Quantum Chemistry*, 121(10):e26614:1–e26614:??, May 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2020:DFT

[TXW+20] Jing Tang, Dong-Hui Xu, Xin Wang, Laicai Li, Xiang-Yang Liu, Xin-Tong Su, Jianmin Guo, and Bin Zhai. A density functional theory study of the stereoselectivity of $Cu(OTf)_2$-catalyzed $[3+2]$ cycloaddition of trifluoromethylated *N*-acylhydrazones and isoprene: a concerted asynchronous mechanism. *International Journal of Quantum Chemistry*, 120(14):e26236:1–e26236:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

tamerd:2022:SES

[tZNb+22] Mohamed Ait tamerd, Mohamed Zanouni, Abdelaziz Nid-bahami, Mustapha Diani, and Adil Marjaoui. Strain effects on the structural, electronic, optical and thermoelectric properties of Si_2SeS monolayer with puckered honeycomb structure: a first-principles study. *International Journal of Quantum Chemistry*, 122(13):e26906:1–e26906:??, July 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uddin:2020:HDR

[UAH+20] Kabir M. Uddin, Ahmad I. Alrawashdeh, David J. Henry, Peter L. Warburton, and Raymond A. Poirier. Hydrolytic deamination reactions of amidine and nucleobase derivatives. *International Journal of Quantum Chemistry*, 120 (1):e26059:1–e26059:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Unal:2020:IWC

[ÜB20] Asli Ünal and Ugur Bozkaya. Ionized water clusters, $(H_2O)_n^+$, $n = 2$ to 6: a high-accuracy study of structures and energetics. *International Journal of Quantum Chemistry*, 120(7):e26100:1–e26100:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uppalapati:2021:STA

[UBV+21] Pramod Kumar Uppalapati, Avni Berisha, Krishnasamy Velmurugan, Raju Nandhakumar, Ajit Khosla, and Tongxiang Liang. Salen type additives as corrosion mitigator for Ni-W alloys: Detailed electronic/atomic-scale computational illustration. *International Journal of Quantum Chemistry*, 121(9):e26600:1–e26600:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ullah:2022:CCD

[UBW+22] Kaleem Ullah, Bakht Amin Bacha, Umer Wahid, Arif Ullah, and Muhammad Irfan. Complex conductivity dependent surface plasmon polaritons at the interface of metal and silver silica nanocomposites. *International Journal of Quantum Chemistry*, 122(3):e26831:1–e26831:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ungordu:2020:EOC

[Üng20] Ayhan Üngördü. Electronic, optical, and charge transfer properties of porphyrin and metallated porphyrins in different media. *International Journal of Quantum Chemistry*, 120(6):e26128:1–e26128:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Umerbekova:2020:MBR

[UP20] Alina Umerbekova and Michele Pavanello. Many-body response of benzene at monolayer MoS_2: van der Waals interactions and spectral broadening. *International Journal of Quantum Chemistry*, 120(21):e26243:1–e26243:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ulian:2020:FPI

[UV20] Gianfranco Ulian and Giovanni Valdrè. First principle investigation of the thermomechanical properties of type A carbonated apatite. *International Journal of Quantum Chemistry*, 120(2):e26069:1–e26069:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:2021:CVE

[Var21] António J. C. Varandas. Canonical versus explicitly correlated coupled cluster: Post-complete-basis-set extrapolation and the quest of the complete-basis-set limit. *International Journal of Quantum Chemistry*, 121(9):e26598:1–e26598:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velasquez:2021:MSB

[VCM+21] Angie Velásquez, Yuly Chamorro, Alejandro Maldonado, Gustavo Aucar, and Albeiro Restrepo. Microsolvation of Sr^{2+}, Ba^{2+}: Structures, energies, bonding, and nuclear magnetic shieldings. *International Journal of Quantum Chemistry*, 121(18):e26753:1–e26753:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ventura:2022:IKS

[VdM22] Elizete Ventura and Silmar A. do Monte. Increasing the kinetic stability of a gas-phase contact ion-pair through enhancement of the carbocation stability. *International Journal of Quantum Chemistry*, 122(12):e26904:1–e26904:??, June 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vlahovic:2020:DFA

[VGSS20] Filip Vlahovic, Maja Gruden, Stepan Stepanovic, and Marcel Swart. Density functional approximations for consistent spin and oxidation states of oxoiron complexes. *International Journal of Quantum Chemistry*, 120(5):e26121:1–e26121:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ventura:2021:SFB

[VKK+21] Oscar N. Ventura, Martina Kieninger, Aline Katz, Mauricio Vega-Teijido, Marc Segovia, and Kenneth Irving. SVECV-f12: Benchmark of a composite scheme for accurate and cost effective evaluation of reaction barriers. *International Journal of Quantum Chemistry*, 121(18):e26745:1–e26745:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vashchenko:2021:SSD

[VKS21] Alexander V. Vashchenko, Anton V. Kuzmin, and Bagrat A. Shainyan. Single Si-doped fullerene as a catalyst in the oxygen reduction reaction: a quantum chemical insight. *International Journal of Quantum Chemistry*, 121(7):e26565:1–e26565:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vassetti:2021:EPD

[VL21] Dario Vassetti and Frédéric Labat. Evaluation of the performances of different atomic charge and nonelectrostatic models in the finite-difference Poisson–Boltzmann approach. *International Journal of Quantum Chemistry*, 121 (7):e26560:1–e26560:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velloso:2020:PIE

[VM20] Paulo F. G. Velloso and José R. Mohallem. Probing internal electric fields of π- and σ-hole bonds. *International Journal of Quantum Chemistry*, 120(5):e26116:1–e26116:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vila-Nadal:2021:PRI

[VN21] Laia Vilà-Nadal. POMzites: a roadmap for inverse design in metal oxide chemistry. *International Journal of Quantum Chemistry*, 121(5):e26493:1–e26493:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vitkovskaya:2020:QCM

[VOK+20] Nadezhda M. Vitkovskaya, Vladimir B. Orel, Vladimir B. Kobychev, Alexander S. Bobkov, Damir Z. Absalyamov, and Boris A. Trofimov. Quantum-chemical models of KOH(KOBu^t)/DMSO superbasic systems and mechanisms of base-promoted acetylene reactions. *International Journal of Quantum Chemistry*, 120(9):e26158:1–e26158:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:2020:ODA

[VP20] António J. C. Varandas and Fernando N. N. Pansini. Optimal diffuse augmented atomic basis sets for extrapolation of the correlation energy. *International Journal of Quantum Chemistry*, 120(7):e26135:1–e26135:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyas:2021:CSA

[VSKG21] Nidhi Vyas, Asmita Sen, Aditya Kumar, and Abhinav Grover. Computational study of ammonia generation by iron(III) and iron(IV) complexes supported by trigonal bipyramidal iron. *International Journal of Quantum Chemistry*, 121(21):e26775:1–e26775:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:NGQ

[WAM+20] LiLing Wang, Alireza Azizi, Roya Momen, Tianlv Xu, Steven R. Kirk, Michael Filatov, and Samantha Jenkins. Next-generation quantum theory of atoms in molecules for the S_1 /S_0 conical intersections in dynamics trajectories of a light-driven rotary molecular motor. *International Journal of Quantum Chemistry*, 120(1):e26062:1–e26062:??, January

1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:ERD

[Wan21] Bin-Bin Wang. Effects of rotational degree of freedom on calculations of photoassociation of HeH^+ systems. *International Journal of Quantum Chemistry*, 121(2):e26426:1–e26426:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2021:TES

[WAW+21] Hua Wu, Mengdi An, Junqing Wen, Lihua Bai, Dongming Li, Jukun Liu, Ruijuan Sun, Wanlin He, Lin Lin, and Yumei Li. Theoretical and experimental studies on concerted elimination of 1, 2-bromochloroethane monocation to $C_2\ H_4^+$ and BrCl. *International Journal of Quantum Chemistry*, 121(2): e26433:1–e26433:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wen:2020:EAA

[WCZ+20] Mingjie Wen, Xiru Cao, Yongqi Zhang, Meng Liang, Tianlei Zhang, Balaganesh Muthiah, Ke Zhou, Soumendra K. Roy, and Makroni Lily. Effect of ammonia, ammonia-water, and sulfuric acid on the $HO_2 + HO_2 \rightarrow H_2O_2 + 3\ O_2$ reaction in troposphere: Competition between stepwise and one-step mechanisms. *International Journal of Quantum Chemistry*, 120(23):e26389:1–e26389:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:EZC

[WDS+20] Kun Wang, Chaohua Dai, Chen Sun, Longjiu Cheng, Jianguo Zhang, and Tonglai Zhang. The effects of Zn^{2+} and ClO_4^- in the excellent primary explosive $Zn(CHZ)_3\ (ClO_4)_2$. *International Journal of Quantum Chemistry*, 120(4):e26107:1–e26107:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weser:2021:CIE

[WFG+21] Oskar Weser, Leon Freitag, Kai Guther, Ali Alavi, and Giovanni Li Manni. Chemical insights into the electronic structure of Fe(II) porphyrin using FCIQMC, DMRG, and generalized active spaces. *International Journal of Quantum*

Chemistry, 121(3):e26454:1–e26454:??, February 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2021:MIL

[WHYL21] Weirong Wu, Hua Hou, Yan Yang, and Tingzhen Li. Mechanistic insight into ligand-promoted C-H alkenylation of arenes with alkynes: a computational study. *International Journal of Quantum Chemistry*, 121(6):e26541:1–e26541:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2021:FSP

[WJF+21] Yong Kai Wei, Liang Quan Jia, Yan Yan Fang, Long Jun Wang, Zhi Xiu Qian, Jiao Nan Yuan, Gurudeeban Selvaraj, Guang Fu Ji, and Dong Qing Wei. Formation and superconducting properties of predicted ternary hydride $ScYH_6$ under pressures. *International Journal of Quantum Chemistry*, 121(4):e26459:1–e26459:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2021:CDS

[WJL+21] Jinting Wu, Yuhe Jiang, Zeng Lian, Hongbo Li, and Jianguo Zhang. Computational design and screening of promising energetic materials: the coplanar family of novel heterocycle-based explosives. *International Journal of Quantum Chemistry*, 121(21):e26788:1–e26788:??, November 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:TMW

[WKH20] Yu-Shu Wang, Sabyasachi Kar, and Yew Kam Ho. Tune-out and magic wavelengths for hydrogenlike and screened-hydrogenlike atoms. *International Journal of Quantum Chemistry*, 120(5):e26115:1–e26115:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2020:MIR

[WLH+20] Weirong Wu, Yue Liu, Jiayi Hu, Jiageng Xiong, and Hua Hou. Mechanistic insight into the rhodium(III)-catalyzed ortho-selective coupling of diverse arenes with 4-acyl-1-sulfonyltriazoles: a computational study. *International Journal of Quantum Chemistry*, 120(3):e26119:1–e26119:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:USE

[WLLS21] Ruijing Wang, Canlin Luo, Qingzhong Li, and Steve Scheiner. Unusual substituent effects in the Tr···Te triel bond. *International Journal of Quantum Chemistry*, 121(6):e26526:1–e26526:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wan:2020:TSP

[WLP+20] Zhehong Wan, Zenan Lin, Jiahui Peng, Wei Chen, Xiaohan Li, and Xiaohui Chen. Theoretical study of propylene epoxidation heterogeneous-homogeneous mechanism over MoO_x /SiO_2 catalyst. *International Journal of Quantum Chemistry*, 120(18):e26328:1–e26328:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:AID

[WLY+20] Jiajun Wang, Shengcai Li, Fengyi Yun, Xin Zhang, and Qunxiang Li. Achieving indirect-to-direct band gap transition and enhanced photocatalytic performance in blue phosphorene through doping and strain. *International Journal of Quantum Chemistry*, 120(13):e26230:1–e26230:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wasserman:2020:QEE

[WP20] Adam Wasserman and Michele Pavanello. Quantum embedding electronic structure methods. *International Journal of Quantum Chemistry*, 120(21):e26495:1–e26495:??, November 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wolinski:2022:CRG

[WP22] Krzysztof Wolinski and Peter Pulay. Compact representation of generalized molecular polarizabilities and efficient calculation of polarization energy in an arbitrary electric field. *International Journal of Quantum Chemistry*, 122(8):

e26792:1–e26792:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:TIM

[WSSD21] Youjia Wang, Yao Shi, Jiaxuan Shao, and Chao Deng. Theoretical insights into the mechanism of rhodium-catalyzed, P^{III} -directed regioselective C–H arylation of indole with anhydride. *International Journal of Quantum Chemistry*, 121(4):e26475:1–e26475:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:CIV

[WV20a] Feng Wang and Vladislav Vasilyev. Cover image, volume 120, issue 23. *International Journal of Quantum Chemistry*, 120(23):e26513:1–e26513:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:MDS

[WV20b] Feng Wang and Vladislav Vasilyev. Molecular dynamics study of ferrocene topology under various temperatures. *International Journal of Quantum Chemistry*, 120(23): e26398:1–e26398:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:AOR

[WV21] Feng Wang and Vladislav Vasilyev. Accelerating optical reporting for conformation of tyrosine kinase inhibitors in solutions. *International Journal of Quantum Chemistry*, 121(20):e26765:1–e26765:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2022:DTM

[WWKH22] Yang Wang, Baisi Wei, Sabyasachi Kar, and Yew Kam Ho. Dipole transition-matrix elements and oscillator strengths for the C^{4+} doubly excited states with Coulomb and screened Coulomb (Debye–Hückel) potentials. *International Journal of Quantum Chemistry*, 122(3):e26833:1–e26833:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wan:2021:APS

[WWL21] Zhongyu Wan, Quan-De Wang, and Jinhu Liang. Accurate prediction of standard enthalpy of formation based on semiempirical quantum chemistry methods with artificial neural network and molecular descriptors. *International Journal of Quantum Chemistry*, 121(2):e26441:1–e26441:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wan:2021:MLP

[WWLL21] Zhongyu Wan, Quan-De Wang, Dongchang Liu, and Jinhu Liang. Machine learning prediction of the optimal carrier concentration and band gap of quaternary thermoelectric materials via element feature descriptors. *International Journal of Quantum Chemistry*, 121(18):e26752:1–e26752:??, September 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:FPSb

[WWM+21] Chao Wang, Jianfeng Wang, Di Ma, Shijie Zhu, Liguo Wang, and Shaokang Guan. First-principles studies on structure stability, segregation, and work function of Mg doped with metal elements. *International Journal of Quantum Chemistry*, 121(11):e26626:1–e26626:??, June 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:SCA

[WWWC21] Peng Wang, Panpan Wu, Kun Wang, and Longjiu Cheng. Stabilization of the [cyclo-N_5]$^-$ anion by Lewis acid-base interactions. *International Journal of Quantum Chemistry*, 121(4):e26473:1–e26473:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:TES

[WWZ+20] Yue Wang, Xingyu Wang, Xiao Zhang, Haolun Fu, Zhaoyang Tan, and Haijun Zhang. Theoretical and experimental studies on the thermal decomposition and fire-extinguishing performance of cis-1,1,1,4,4,4-hexafluoro-2-butene. *International Journal of Quantum Chemistry*, 120 (9):e26160:1–e26160:??, May 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:OEE

[WWZ+21] Xiangqian Wang, Haiyan Wang, Lifeng Zheng, Chun Zhu, and Jin-Xia Liang. Oriented external electric fields regulating the oxidation reaction of CH_4 catalyzed by Mncorrolazine. *International Journal of Quantum Chemistry*, 121(2):e26443:1–e26443:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:FPSa

[WXL+21] Jiao Wang, Zhiguo Xing, Zhenlin Lu, Kaining Ding, and Haidou Wang. First-principle study of the properties in $BaTiO_3$ and the electronic structure of H_2 O adsorption on $BaTiO_3$. *International Journal of Quantum Chemistry*, 121 (8):e26576:1–e26576:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:CEB

[WXLL21] Ruijng Wang, Bo Xiao, Wenzuo Li, and Qingzhong Li. Cooperative effects between triel and halogen bonds in complexes of pyridine derivatives: an opposite effect of the nitrogen oxidation on triel and halogen bonds. *International Journal of Quantum Chemistry*, 121(2):e26429:1–e26429:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:SCH

[WY20] Li-Zhi Wang and Chuan-Lu Yang. Stereodynamics of the Ca + HCl $\rightarrow$ CaCl + H molecular reaction imposed by the rotational-excited states of HCl. *International Journal of Quantum Chemistry*, 120(24):e26411:1–e26411:??, December 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:CEI

[WYZZ20] Guangfu Wang, Lixia Yan, Shahid Zaman, and Minjie Zhang. The connective eccentricity index of graphs and its applications to octane isomers and benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, 120(18):e26334:1–e26334:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2020:EOE

[WZ20] Wenjing Wang and Shaohui Zheng. Exploring odd–even effects of simple oligomer-like DRCNnT series: a study based on density functional theory/time-dependent density functional theory calculations. *International Journal of Quantum Chemistry*, 120(2):e26066:1–e26066:??, January

15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2021:DRM

[WZ21] Zhen-Yu Wu and Hong Zhang. The different resonant modes for the special 2D/1D hybrid structures in the visible-light region. *International Journal of Quantum Chemistry*, 121 (7):e26550:1–e26550:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2021:IHN

[WZL+21] Rui Wang, Yongqi Zhang, Aizhen Li, Mingjie Wen, Zerong Geng, Ximei Geng, Zhuqing Wang, Zhiyin Wang, and Makroni Lily. Influence of H_2 O and NH_3 on the reaction of HO_2 with NO in troposphere: Theoretical investigation of HNO_3 formation pathways. *International Journal of Quantum Chemistry*, 121(2):e26432:1–e26432:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xing:2022:CHC

[XAM+22] Hui Xing, Alireza Azizi, Roya Momen, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. Chirality-helicity of cumulenes: a non-scalar charge density derived perspective. *International Journal of Quantum Chemistry*, 122(10):e26884:1–e26884:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2020:FRW

[XBK+20] Tianlv Xu, Xin Bin, Steven R. Kirk, David J. Wales, and Samantha Jenkins. Flip rearrangement in the water pentamer: Analysis of electronic structure. *International Journal of Quantum Chemistry*, 120(6):e26124:1–e26124:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2021:FPS

[XCZ+21] Wenhui Xu, Yuhong Chen, Yingjie Zhao, Meiling Zhang, Ranran Tian, and Cairong Zhang. First-principles study on the methane adsorption properties by Ti-modified graphyne. *International Journal of Quantum Chemistry*, 121 (24):e26811:1–e26811:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiao:2020:HTF

[XFW+20] Hui Xiao, Touwen Fan, Zhipeng Wang, Te Hu, Xian Tang, Li Ma, and Pingying Tang. High-throughput first-principle calculations of the structural, mechanical, and electronic properties of cubic $XTiO_3$ (X = Ca, Sr, Ba, Pb) ceramics under high pressure. *International Journal of Quantum Chemistry*, 120(10):e26168:1–e26168:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2020:TSB

[XHX+20] Chengcheng Xu, Xinyue Huang, Xin Xu, Xiao Zhang, and Haijun Zhang. Theoretical studies on the BC_2N monolayers with promising photoelectronic characteristics and remarkable environmental stabilities. *International Journal of Quantum Chemistry*, 120(6):e26120:1–e26120:??, March 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2020:IME

[XJ20] Bin-Jie Xie and Chun-Sheng Jia. Improved multiparameter exponential-type potential for diatomic molecules. *International Journal of Quantum Chemistry*, 120(1):e26058:1–e26058:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2021:HPC

[XJLH21] Hui Hui Xie, Li Guang Jiao, Aihua Liu, and Yew Kam Ho. High-precision calculation of relativistic corrections for hydrogen-like atoms with screened Coulomb potentials. *International Journal of Quantum Chemistry*, 121(13):e26653:1–e26653:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiang:2020:TSP

[XPZ20] Yunjie Xiang, Suoping Peng, and Shaohui Zheng. Theoretical studies of photovoltaic properties of five new silol dithiophene based D_2-A-D_1-A-D_2 donors. *International Journal of Quantum Chemistry*, 120(1):e26047:1–e26047:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2021:ERT

[XQJ+21] Shaohua Xu, Gangqiang Qin, Quan Jiang, Qianyi Cui, Aijun Du, Chongjun Zhao, and Qiao Sun. N_2 electrochemical reduction on two dimensional transition metal monoborides: a density functional theory study. *International Journal of Quantum Chemistry*, 121(7):e26548:1–e26548:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2021:CFB

[XWJ+21] Jin Xu, Jinting Wu, Yuhe Jiang, Lian Zeng, Wei Li, Ming Huang, Hongbo Li, and Jianguo Zhang. The coplanar family of bis(nitrotriazoles) tetrazine and oxides based as energetic compounds. *International Journal of Quantum Chemistry*, 121(2):e26364:1–e26364:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2020:MDN

[XWLZ20] Jin Xu, Jinting Wu, Hongbo Li, and Jianguo Zhang. Molecular design of a new family of bridged bis(multinitro-triazole) with outstanding oxygen balance as high-density energy compounds. *International Journal of Quantum Chemistry*, 120(1):e26056:1–e26056:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2022:DFT

[XWS+22] Shuo Xu, Shi-Jie Wang, Wan-Qi Sun, Xiao-Hong Li, and Hong-Ling Cui. Density functional theory study of the electronic properties and quantum capacitance of pure and doped Zr_2CO_2 as electrode of supercapacitors. *International Journal of Quantum Chemistry*, 122(4):e26844:1–e26844:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2020:DND

[XZ20] Xiaoping Xu and Shaohui Zheng. Designing new donor materials based on functionalized DCCnT with different electron-donating groups: a density functional theory (DFT) and time dependent density functional theory (TDDFT)-based study. *International Journal of Quantum Chemistry*, 120(8):e26112:1–e26112:??, April 15, 2020. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2020:IPS

[Yan20] Xiao-Yong Yang. Is it possible to synthesize MNg_2^{2+} $(Sb_2F_{11}^{-1})_2$ (Ng = Ar, He, He; M = Au, Ga, Cu) bulk salt compounds? *International Journal of Quantum Chemistry*, 120(16):e26246:1–e26246:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2021:MBL

[Yan21] Lijuan Yan. The magnetic binary lithium clusters W_2 Li_n (n = 15-19): a theoretical prediction of “di-superatomic molecules”. *International Journal of Quantum Chemistry*, 121(2):e26434:1–e26434:??, January 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakar:2021:ESO

[YÇDÖ21] Yusuf Yakar, Bekir Çakir, Celalettin Demir, and Ayhan Özmen. Energy states, oscillator strengths and polarizabilities of many electron atoms confined by an impenetrable spherical cavity. *International Journal of Quantum Chemistry*, 121(13):e26658:1–e26658:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yong:2022:PIE

[YCL+22] Yik Seng Yong, Yee Hui Robin Chang, Lay Chen Low, Thong Leng Lim, and Tiem Leong Yoon. Pressure-induced enhancement of mechanical performance in ZrC system. *International Journal of Quantum Chemistry*, 122(11): e26897:1–e26897:??, June 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2020:ESC

[YCPW20] Qiang Yang, Xing Hong Cai, Yong Pang, and Min Wang. The effects of strain and charge doping on the electronic properties of graphitic C_3 N_5. *International Journal of Quantum Chemistry*, 120(22):e26378:1–e26378:??, November 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yusupova:2020:SAR

[YCSK20] Alfia R. Yusupova, Ekaterina M. Chainikova, Rustam L. Safiullin, and Sergey L. Khursan. Structure-activity relationship in the case of intramolecular ortho -cyclization of aromatic nitroso oxides: Inverted steric effect of substituent in the 2-R-C_6H_4 NOO transformation. *International Journal of Quantum Chemistry*, 120(4):e26094:1–e26094:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ye:2020:EWK

[Ye20] Luzhen Ye. Extremal Wiener and Kirchhoff indices of globular caterpillars. *International Journal of Quantum Chemistry*, 120(4):e26096:1–e26096:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yongmei:2022:AES

[YFX+22] Zhang Yongmei, Wang Furong, Wang Xiaona, Zhao Huifang, Zhang Xiuqing, and Gao Yanqin. Anisotropy in elasticity, sound velocity, thermal conductivity, and thermodynamics properties of dodecaboride $Zr_{0.5}Y_{0.5}B_{12}$. *International Journal of Quantum Chemistry*, 122(3):e26836:1–e26836:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2022:DSF

[YHW+22] Rourou Yu, Wenhao Hu, Xingyu Wang, Xiao Zhang, and Zhaoyang Tan. In depth study on the fire-extinguishing mechanism of Octafluoro-2-butene as a new promising Halon substitute. *International Journal of Quantum Chemistry*, 122(14):e26913:1–e26913:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2022:TDF

[YHZ+22] Rourou Yu, Wenhao Hu, Xiao Zhang, Xingyu Wang, and Zhaoyang Tan. Thermal decomposition and fire-extinguishing mechanism of CF_3I: a combined theoretical and experimental study. *International Journal of Quantum Chemistry*, 122(4):e26845:1–e26845:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2020:EHR

[YLL+20] Jieqiong Yang, Dongzhi Liu, Ting Lu, Haiya Sun, Wei Li, Thomas T. Testoff, Xueqin Zhou, and Lichang Wang. Effects of heterocyclic ring and amino-ethyl-amino group on the electronic and photophysical properties of a triphenylamine-pyrimidine dye. *International Journal of Quantum Chemistry*, 120(19):e26355:1–e26355:??, October 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshizawa:2020:MDP

[Yos20] Terutaka Yoshizawa. A mathematical discussion of Pons Viver's implementation of Löwdin's spin projection operator. *International Journal of Quantum Chemistry*, 120(12): e26215:1–e26215:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Pon19].

Yao:2021:BRA

[YST+21] Junfang Yao, Yanan Sun, Yizhen Tang, Yunju Zhang, Wenzhong Wu, and Jingyu Sun. Book review: *Atmospheric oxidation of 4-(2-methoxyethyl) phenol initiated by OH radical in the presence of O_2 and NO_x: a mechanistic and kinetic study*. *International Journal of Quantum Chemistry*, 121 (13):e26650:1–e26650:??, July 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2021:BFT

[YXKJ21] Yong Yang, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. Bond flexing, twisting, anharmonicity and responsivity for the infrared-active modes of benzene. *International Journal of Quantum Chemistry*, 121(8):e26584:1–e26584:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yun:2021:TIR

[YYL21] Xiao Yun, Zhangyu Yu, and Tao Liu. Theoretical investigation on the rhodium-catalyzed coupling reaction of ketoxime with 1,3-enynes: $[4+1]$ vs $[4+2]$ annulation. *International Journal of Quantum Chemistry*, 121(4):e26449:1–e26449:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2020:MKE

[YZD+20] Yu-Qi Yang, Wei Zhang, Ming-Shuai Deng, Xiu-Mei Pan, Feng-Yang Bai, and Lei Tan. Mechanism, kinetics, and environmental assessment of OH-initiated transformation of CTDE in the atmosphere. *International Journal of Quantum Chemistry*, 120(15):e26250:1–e26250:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2021:HPE

[YZD+21] Fangqian Yin, Tingchun Zhu, Chunhua Dong, Bin Li, and Le Zhang. H_2 promoting effect in Cr/PNP-catalyzed ethylene tetramerization: a density functional theory study. *International Journal of Quantum Chemistry*, 121(15): e26667:1–e26667:??, August 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2021:EMT

[YZL21a] Li-Hua Yao, Jian-Guo Zhao, and Jing-Wei Li. Effects of microstructural tailoring on Na storage performance of graphene. *International Journal of Quantum Chemistry*, 121 (14):e26660:1–e26660:??, July 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2021:FPS

[YZL+21b] Xinyan Yu, Hongliang Zhang, Jie Li, Hui Guo, Jingkun Wang, Jiacheng Wang, and Mengqiu Long. First-principles study of the adsorption mechanism of SO_2 and CF_4 on the α-Al_2O_3 (0001) surface. *International Journal of Quantum Chemistry*, 121(5):e26507:1–e26507:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2022:EMP

[YZY+22] Guang Yang, Huiyang Zhang, Yijun Yang, Yudi Wang, Xinzi Xv, Xinli Zhao, Lijuan Meng, Xiaojing Yao, Xiuyun Zhang, and Yongjun Liu. Electronic and magnetic properties of one-dimensional sandwich transition metal-anthracene molecular wires. *International Journal of Quantum Chemistry*, 122(3):e26832:1–e26832:??, February 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2022:FDE

[ZCL+22] Cai-Rong Zhang, Hong Chen, Zi-Jiang Liu, Mei-Ling Zhang, Wei Wang, You-Zhi Wu, and Hong-Shan Chen. Formamidinium dopant effects on double perovskite $Cs_2AgBiBr_6$. *International Journal of Quantum Chemistry*, 122(4): e26846:1–e26846:??, February 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:SSB

[ZFB+20] Li-Juan Zhang, Lin-Yan Feng, He Bian, Ling Pei, Da-Zhi Li, and Hua-Jin Zhai. In search of the smallest boroxol-type heterocyclic ring system: Planar hexagonal $B_3S_3^+$ cluster with double $6\pi/2\sigma$ aromaticity. *International Journal of Quantum Chemistry*, 120(13):e26229:1–e26229:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2021:GOC

[ZG21] Jun Zhang and Vassiliki-Alexandra Glezakou. Global optimization of chemical cluster structures: Methods, applications, and challenges. *International Journal of Quantum Chemistry*, 121(7):e26553:1–e26553:??, April 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2020:EES

[ZGCF20] Shuangfei Zhu, Qiang Gan, Nianshou Cheng, and Changgen Feng. Exploring the effects of solvents on an organic explosive: Insights from the electron structure, electrostatic potential, and conformational transformations of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane. *International Journal of Quantum Chemistry*, 120(12): e26202:1–e26202:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:LDH

[ZGJ+20] Yong Zhi Zhang, Ya Chen Gao, Li Guang Jiao, Fang Liu, and Yew Kam Ho. Linear dependence in Hylleraas configuration-interaction calculations of He atom. *International Journal of Quantum Chemistry*, 120(7):e26136:1–e26136:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zuluaga-Hernandez:2020:OEP

[ZHFD+20] Edison A. Zuluaga-Hernández, Elizabeth Flórez, Ludovic Dorkis, Miguel E. Mora-Ramos, and Julian D. Correa. Opto-electronic properties of blue phosphorene oxide with and without oxygen vacancies. *International Journal of Quantum Chemistry*, 120(2):e26075:1–e26075:??, January 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2020:RGP

[ZHJ+20] Lin Zhu, Yu Ying He, Li Guang Jiao, Yuan Cheng Wang, and Yew Kam Ho. Revisiting the generalized pseudospectral method: Radial expectation values, fine structure, and hyperfine splitting of confined atom. *International Journal of Quantum Chemistry*, 120(14):e26245:1–e26245:??, July 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zokaie:2021:MKR

[ZHS21] Meymanat Zokaie, S. Rasoul Hashemi, and Vahid Saheb. Mechanism and kinetics of the reaction CH_3 + CH_3CHO: Ab initio semiclassical transition state theory study. *International Journal of Quantum Chemistry*, 121(4):e26468:1–e26468:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2021:EUH

[Zhu21] Qiangyuan Zhu. Extremal k-uniform hypertrees on incidence energy. *International Journal of Quantum Chemistry*, 121(9):e26592:1–e26592:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2020:EPE

[ZIA20] Anton B. Zakharov, Vladimir V. Ivanov, and Ludwik Adamowicz. Electronic perturbation effects in the presence of electric field for π-conjugated systems: an electron-correlation study. *International Journal of Quantum Chemistry*, 120(16):e26260:1–e26260:??, August 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2021:CIS

[ZJW+21] Lian Zeng, Yuhe Jiang, Jinting Wu, Hongbo Li, and Jianguo Zhang. Computational investigation and screening of high-energy-density materials: Based on nitrogen-rich 1,2,4,5-tetrazine energetic derivatives. *International Journal of Quantum Chemistry*, 121(17):e26742:1–e26742:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2022:NID

[ZKP22] Yuming Zhao and Cody Marcus King-Poole. Noncovalent interactions of 1,4-dithiafulvene and nitroaromatics: a combined DFT and ab initio molecular dynamics (AIMD) study. *International Journal of Quantum Chemistry*, 122 (10):e26887:1–e26887:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2021:TSH

[ZL21] Lijuan Zhang and Dazhi Li. Theoretical studies on how to tune the π-hole pnicogen bonds by substitution and cooperative effects. *International Journal of Quantum Chemistry*, 121(6):e26531:1–e26531:??, March 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:MSP

[ZLH20a] Yujin Zhang, Jiancai Leng, and Wei Hu. A multiscale study on photophysical properties of a novel fluorescent probe for imaging amyloid-β in Alzheimer's disease. *International Journal of Quantum Chemistry*, 120(18):e26344:1–e26344:??, September 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2020:ISE

[ZLH+20b] Yunxuan Zhou, Qianli Liu, Mingyu Hu, Gengsen Xu, Ruiju Xu, Xiaoyu Chong, and Jing Feng. Investigation on the stability, electronic, optical, and mechanical properties of novel calcium carbonate hydrates via first-principles calculations. *International Journal of Quantum Chemistry*, 120 (10):e26219:1–e26219:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:HPC

[ZLT+20] Zhong Zhang, Chencheng Liu, Ge Tian, Zuqing Chen, Liang Pu, and Robert Bruce King. The heavier pnictogen and chalcogen analogues of isocyanic and cyanic acids and their dimers: a high level ab initio study. *International Journal of Quantum Chemistry*, 120(1):e25989:1–e25989:??, January 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:GIA

[ZMJ+20] Baohua Zhang, Yingjin Ma, Xinsheng Jin, Ying Wang, Bingbing Suo, Xiao He, and Zhong Jin. GridMol2.0: Implementation and application of linear-scale quantum mechanics methods and molecular visualization. *International Journal of Quantum Chemistry*, 120(23):e26402:1–e26402:??, December 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zobair:2021:EBT

[ZMS21] Mian Muhammad Zobair, Mehar Ali Malik, and Hani Shaker. Eccentricity-based topological invariants of tightest nonadjacently configured stable pentagonal structure of carbon nanocones. *International Journal of Quantum Chemistry*, 121(24):e26807:1–e26807:??, December 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zueva:2020:IIT

[ZPS+20] Ekaterina M. Zueva, Maria M. Petrova, Aliia V. Shamsieva, Kamila R. Trigulova, Elvira I. Musina, Robert R. Fayzullin, Artem S. Bogomyakov, Victor I. Ovcharenko, and Andrey A. Karasik. Insight into the influence of terminal ligands on magnetic exchange coupling in a series of dimeric copper(II) acetate adducts. *International Journal of Quantum Chemistry*, 120(8):e26145:1–e26145:??, April 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zerrouki:2021:FPC

[ZRR+21] Tayeb Zerrouki, Habib Rached, Djamel Rached, Messaoud Caid, Oualid Cheref, and Mohamed Rabah. First-principles calculations to investigate structural stabilities, mechanical and optoelectronic properties of NbCoSn and NbFeSb half-Heusler compounds. *International Journal of Quantum Chemistry*, 121(8):e26582:1–e26582:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2021:NIS

[ZS21] Qianlong Zhou and Bingbing Suo. New implementation of spin-orbit coupling calculation on multi-configuration electron correlation theory. *International Journal of Quantum Chemistry*, 121(20):e26772:1–e26772:??, October 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2022:TEB

[ZWL22] Yiying Zhang, Shouqiang Wu, and Anyong Li. Theoretically exploring the bonding properties of trivalent transuranic elements with 2-(2-amino-2-oxyethoxy) acetic acid. *International Journal of Quantum Chemistry*, 122(14):e26914:1–e26914:??, July 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2022:MSP

[ZWW+22] Yanliang Zhao, Honglei Wang, Naiwei Wu, Junxia Yang, Jikai Sun, Dong Zhai, and Weiqiao Deng. The mechanism of sugar produced from simple glycolaldehyde derivative at ambient conditions. *International Journal of Quantum Chemistry*, 122(7):e26865:1–e26865:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2021:MLL

[ZX21] Yun Zhang and Xiaojie Xu. Machine learning lattice parameters of monoclinic double perovskites. *International Journal of Quantum Chemistry*, 121(5):e26480:1–e26480:??, March 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:EEF

[ZXS20] Ming-Xia Zhang, Hong-Liang Xu, and Zhong-Min Su. External electric field-phenyl interaction boosts hydrosilylation of substituted alkynes to α-vinylsilane. *International Journal of Quantum Chemistry*, 120(7):e26134:1–e26134:??, April 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2021:NOP

[ZXS21] Feng-Yi Zhang, Hong-Liang Xu, and Zhong-Min Su. The nonlinear optics property of heterodinuclear (Li and Na) sexipyridine helix: a density functional theory study. *International Journal of Quantum Chemistry*, 121(4):e26478:1–e26478:??, February 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2021:CUO

[ZYZ+21a] Li Zhang, Ya-Ling Ye, Xiao-Ling Zhang, Xiang-Hui Li, Qiao-Hong Chen, Jing-Hua Chen, and Wei-Ming Sun. Cisplatin under oriented external electric fields: a deeper insight into electrochemotherapy at the molecular level. *International Journal of Quantum Chemistry*, 121(8):e26578:1–e26578:??, April 15, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2021:SIL

[ZYZ+21b] Chuan-Zhen Zhao, Huang Yu, Min-Min Zhu, Si-Yu Sun, and Yu Guo. Sulfur impurity level in the O-rich ZnS_xO_{1-x} alloy obtained by first principle calculations. *International Journal of Quantum Chemistry*, 121(9):e26604:1–e26604:??, May 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2022:ARP

[ZYZ+22] Wenna Zhang, Tong Yang, Kristin Zhao, Xiaobin Liao, and Yan Zhao. Accurate redox potentials for solvents in Li-metal batteries and assessment of density functionals. *International Journal of Quantum Chemistry*, 122(10):e26886:1–e26886:??, May 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2022:EHM

[ZZ22] Guojia Zhu and Shaohui Zheng. Exploring the hole mobility of oligothiophene based donors with different spatial symmetry and conjugation length of backbone: a theoretical insight. *International Journal of Quantum Chemistry*, 122 (1):e26820:1–e26820:??, January 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2022:SCB

[ZZF22] Lili Zhao, Minna Zhi, and Gernot Frenking. The strength of a chemical bond. *International Journal of Quantum Chemistry*, 122(8):e26773:1–e26773:??, April 15, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2020:MHD

[ZZL+20a] Hongxia Zhou, Fayan Zhu, Hongyan Liu, Wenqian Zhang, Yongquan Zhou, and Chunhui Fang. Mechanism for hydrolysis of double six-membered ring tetraborate anion. *International Journal of Quantum Chemistry*, 120(5):e26118:1–e26118:??, March 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zou:2020:ESU

[ZZL20b] Xin Zou, Zhongxun Zhu, and Hongyan Lu. The extremal structures of k-uniform unicyclic hypergraphs on Wiener index. *International Journal of Quantum Chemistry*, 120(3): e26091:1–e26091:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:TDD

[ZZLC20] Bofeng Zhang, Hong Zhang, Jiahe Lin, and Xinlu Cheng. A time-dependent density functional study on optical response in all-inorganic lead-halide perovskite nanostructures. *International Journal of Quantum Chemistry*, 120(13):e26232:1–e26232:??, July 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2022:TST

[ZZLY22] Qiong Zhu, Panwang Zhou, Jianyong Liu, and Shuhui Yin. Theoretical study on the thermal dissociation of FOX-7 promoted by NO_2. *International Journal of Quantum Chemistry*, 122(7):e26864:1–e26864:??, April 5, 2022. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2021:MDL

[ZZXT21] Xiuxiu Zhao, Yingchao Zhang, Congxia Xie, and Long Tan. Molecular design of long intra-annular nitrogen chains: 3H-tetrazolo[1,5-d]tetrazole-based high-energy-density materials. *International Journal of Quantum Chemistry*, 121(17):

e26743:1–e26743:??, September 5, 2021. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:DFT

[ZZZ+20a] Shiguo Zhang, Yan Zhang, Yun Zhang, Ziyan Feng, Caihong Wang, He Bian, and Jinshe Chen. A density functional theory study on the atmospheric reaction of CH_3O_2 with HS: Mechanism and kinetics. *International Journal of Quantum Chemistry*, 120(17):e26330:1–e26330:??, September 1, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2020:ESD

[ZZZ20b] Ben-Chao Zhu, Shuai Zhang, and Lu Zeng. The effect of silicon doping on the geometrical structures, stability, and electronic and spectral properties of magnesium clusters: DFT study of $SiMg_n$ ($n = 1$–12) clusters. *International Journal of Quantum Chemistry*, 120(10):e26143:1–e26143:??, May 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2020:CSR

[ZZZW20] Jing Zhang, Qingli Zhang, Zhenyuan Zhu, and Bingkai Wang. Computational study on the Rh-catalyzed chemodivergent oxidative annulation of benzamides and enynes. *International Journal of Quantum Chemistry*, 120(15): e26252:1–e26252:??, August 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).