

Publication List

- [1] J. M. S. Law, M. Szori, R. Izsak, B. Penke, I. G. Csizmadia and B. Viskolcz, Folded and unfolded conformations of the omega-3 polyunsaturated fatty acid acid family: $\text{CH}_3\text{CH}_2[\text{CH}=\text{CHCH}_2]_B[\text{CH}_2]_M\text{COOH}$. First Principles Study, *J. Phys. Chem. A*, 2006, **110**, 6100.
- [2] G. Tasi, R. Izsak, G. Matisz, A. G. Csaszar, M. Kallay, B. Ruscic and J. F. Stanton, The origin of systematic error in the standard enthalpies of formation of hydrocarbons computed via atomization schemes, *ChemPhysChem*, 2006, **7**, 1664.
- [3] R. Izsak, B. Jojart, I. G. Csizmadia and B. Viskolcz, Role of aromaticity, ring strain, and stereochemistry of selected disulfides and their congeners in the oxidative linkage of DNA Strands at the major groove. A computational study, *J. Chem. Inf. Model.*, 2006, **46**, 2527.
- [4] B. Viskolcz, M. Szori, R. Izsak, S. N. Fejer and I. G. Csizmadia, Thermodynamic functions of conformational changes, Part IV: Functional analysis of conformational entropy of substituted ethane and methanol, *Int. J. Quant. Chem.*, 2007, **107**, 1826.
- [5] R. Izsák, M. Szóri, P. J. Knowles and B. Viskolcz, High Accuracy ab Initio Calculations on Reactions of OH with 1-Alkenes. The Case of Propane, *J. Chem. Theory Comput.*, 2009, **5**, 2313.
- [6] M. Szóri, B. Jójárt, R. Izsák, K. Szóri, I. G. Csizmadia and B. Viskolcz, Chemical evolution of biomolecule building blocks. Can thermodynamics explain the accumulation of glycine in the prebiotic ocean?, *Phys. Chem. Chem. Phys.*, 2011, **13**, 7449.
- [7] B. Fiser, M. Szori, B. Jojart, R. Izsak, I. G. Csizmadia and B. Viskolcz, Antioxidant Potential of Glutathione: A Theoretical Study, *J. Phys. Chem. B*, 2011, **115**, 11269.
- [8] B. Jójárt, M. Szóri, R. Izsák, I. Marsi, B. Viskolcz and I. G. Csizmadia, The effect of a Pro²⁸Thr point mutation on the local structure and stability of human galactokinase enzyme—a theoretical study, *J. Mol. Mod.*, 2011, **17**, 2639.
- [9] R. Izsák and F. Neese, An overlap fitted chain of spheres exchange method, *J. Chem. Phys.*, 2011, **135**, 144105.
- [10] M.-E. Pandelia, D. Bykov, R. Izsák, P. Infossi, M.-T. Giudici-Orticoni, E. Bill, F. Neese and W. Lubitz, Electronic structure of the unique [4Fe-3S] cluster in O₂-tolerant hydrogenases characterized by ⁵⁷Fe Mössbauer and EPR spectroscopy, *PNAS*, 2012, **110**, 483.
- [11] R. Izsák, A. Hansen and F. Neese, The resolution of identity and chain of spheres approximations for the LPNO-CCSD singles Fock term, *Mol. Phys.*, 2012, **110**, 2413.
- [12] M.-E. Pandelia, D. Bykov, R. Izsák, P. Infossi, M.-T. Giudici-Orticoni, E. Bill, F. Neese and W. Lubitz, Reply to Mouesca et. al.: Electronic structure of the proximal [4Fe-3S] cluster of O₂-tolerant [NiFe] hydrogenases, *PNAS*, 2013, **110**, E2539.
- [13] R. Izsák and F. Neese, Speeding up spin-component-scaled third-order perturbation theory with the chain of spheres approximation: The COSX-SCS-MP3 method, *Mol. Phys.*, 2013, **111**, 1190.
- [14] D. G. Liakos, R. Izsák, F. Neese and E. F. Valeev, What is the most efficient way to reach the canonical MP2 basis set limit?, *Mol. Phys.*, 2013, **111**, 2653.
- [15] R. Izsák, F. Neese and W. Klopper, Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space, *J. Chem. Phys.*, 2013, **139**, 094111.
- [16] P. Merlot, R. Izsák, A. Borgoo, T. Kjærgaard, T. Helgaker and S. Reine, Charge-constrained auxiliary-density-matrix methods for the Hartree-Fock exchange contribution, *J. Chem. Phys.*, 2014, **141**, 094104.
- [17] M. J. Ryding, R. Izsák, P. Merlot, S. Reine, T. Helgaker and E. Uggerud, Geometry of the magic number H⁺(H₂O)₂₁ water cluster by proxy, *Phys. Chem. Chem. Phys.*, 2015, **17**, 5466.

- [18] D. Bykov, T. Petrenko, R. Izsák, S. Kossmann, U. Becker, E. Valeev and F. Neese, Efficient implementation of the analytic second derivatives of Hartree–Fock and hybrid DFT energies: a detailed analysis of different approximations, *Mol. Phys.*, 2015, **113**, 1961.
- [19] A. K. Dutta, F. Neese and R. Izsák, Speeding up Equation of Motion Coupled Cluster Theory with the Chain of Spheres Approximation, *J. Chem. Phys.*, 2016, **144**, 034102.
- [20] E. Rebolini, R. Izsák, S. S. Reine, T. Helgaker and T. B. Pedersen, Comparison of Three Efficient Approximate Exact-Exchange Algorithms: The Chain-of-Spheres Algorithm, Pair-Atomic Resolution-of-the-Identity Method, and Auxiliary Density Matrix Method, *J. Chem. Theory Comput.*, 2016, **12**, 3514.
- [21] A. K. Dutta, F. Neese and R. Izsák, Towards a pair natural orbital coupled cluster method for excited states, *J. Chem. Phys.*, 2016, **145**, 034102.
- [22] A. K. Dutta, M. Nooijen, F. Neese and R. Izsák, Automatic active space selection for the similarity transformed equations of motion coupled cluster method, *J. Chem. Phys.*, 2017, **146**, 074103.
- [23] A. K. Dutta, F. Neese and R. Izsák, A simple scheme for calculating approximate transition moments within the equation of motion expectation value formalism, *J. Chem. Phys.*, 2017, **146**, 214111.
- [24] L. M. J. Huntington, M. Krupička, F. Neese and R. Izsák, Similarity transformed equation of motion coupled-cluster theory based on an unrestricted Hartree-Fock reference for applications to high-spin open-shell systems, *J. Chem. Phys.*, 2017, **147**, 174104.
- [25] A. K. Dutta, F. Neese and R. Izsák, Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation, *Mol. Phys.*, 2018, **116**, 1428.
- [26] A. K. Dutta, M. Nooijen, F. Neese and R. Izsák, Exploring the Accuracy of a Low Scaling Similarity Transformed Equation of Motion Method for Vertical Excitation Energies, *J. Chem. Theory Comput.*, 2018, **14**, 72.
- [27] G. L. Stoychev, A. A. Auer, R. Izsák and F. Neese, Self-consistent field calculation of nuclear magnetic resonance chemical shielding constants using gauge-including atomic orbitals and approximate two-electron integrals, *J. Chem. Theory Comput.*, 2018, **14**, 619.
- [28] B. de Souza, F. Neese and R. Izsák, On the theoretical prediction of fluorescence rates from first principles using the path integral approach, *J. Chem. Phys.*, 2018, **148**, 034104.
- [29] A. K. Dutta, M. Saitow, C. Riplinger, F. Neese and R. Izsák, A near-linear scaling equation of motion coupled cluster method for ionized states, *J. Chem. Phys.*, 2018, **148**, 244101.
- [30] C. E. Schulz, A. K. Dutta, R. Izsák and D. A. Pantazis, Systematic High-Accuracy Prediction of Electron Affinities for Biological Quinones, *J. Comput. Chem.*, 2018, **39**, 2439.
- [31] A. Sen, B. de Souza, L. M. J. Huntington, M. Krupička, F. Neese and R. Izsák, An Efficient Pair Natural Orbital Based Configuration Interaction Scheme for the Calculation of Open-Shell ionization potentials, *J. Chem. Phys.*, 2018, **149**, 114108.
- [32] B. de Souza, G. Farias, F. Neese and R. Izsák, Predicting phosphorescence rates of light organic molecules using TD-DFT and the path integral approach to dynamics, *J. Chem. Theory Comput.*, 2019, **15**, 1896.
- [33] S. Haldar, C. Riplinger, B. Demoulin, F. Neese, R. Izsák and A. K. Dutta, A Multi-layer approach to IP-EOM-DLPNO-CCSD Method: Theory, Implementation and Application, *J. Chem. Theory Comput.*, 2019, **15**, 2265.
- [34] C. Salla, G. Farias, J. Teixeira, A. Bortoluzzi, S. Curcio, T. Cazati, R. Izsák, F. Neese, B. de Souza and I. Bechtold, New Boron(III) blue emitters for all-solution processed OLEDs: molecular design assisted by theoretical modeling, *Eur. J. Inorg. Chem.*, 2019, **2019**, 2247.

- [35] A. K. Dutta, M. Saitow, B. Demoulin, F. Neese and R. Izsák, A domain-based pair natural orbital implementation of the equation of motion coupled cluster method for electron attached states, *J. Chem. Phys.*, 2019, **150**, 164123.
- [36] B. de Souza, G. Farias, F. Neese and R. Izsák, Efficient simulation of overtones and combination bands in Resonant Raman spectra, *J. Chem. Phys.*, 2019, **150**, 214102.
- [37] A. Dittmer, R. Izsák, D. Maganas and F. Neese, An Accurate protocol for the prediction of Band Gap energies of Semiconductors in the Framework of Similarity Transformed Equation of Motion Couple Cluster Theory, *Inorg. Chem.*, 2019, *published online*.
- [38] R. Berraud-Pache, G. Bistoni, F. Neese and R. Izsák, Exploring new near-infrared aza-boron dipyrromethene dyes using a highly accurate novel wavefunction approach, *to be submitted*.
- [39] A. K. Dutta, M. Saitow, B. Demoulin, F. Neese and R. Izsák, A domain-based pair natural orbital implementation of the similarity transformed equation of motion coupled cluster method, *J. Chem. Phys.*, *to be submitted*.