# Dispersion-Corrected Mean-Field Electronic Structure M

Chemical Reviews

116, 5105-5154

DOI: 10.1021/acs.chemrev.5b00533

Citation Report

| # | Article | IF | Citations |
|---|---|---|---|
| 22 | Halogen bonded supramolecular capsules: a challenging test case for quantum chemical methods. Chemical Communications, 2016, 52, 9893-9896. | 2.2 | 26 |
| 23 | Intermolecular dissociation energies of dispersively bound 1-naphtholâ‹…cycloalkane complexes. Journal of Chemical Physics, 2016, 145, 244314. | 1.2 | 11 |
| 24 | Communication: Physical origins of ionization potential shifts in mixed carboxylic acids and water complexes. Journal of Chemical Physics, 2016, 145, 051101. | 1.2 | 6 |
| 25 | Water adsorption on bimetallic PtRu/Pt(111) surface alloys. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160618. | 1.0 | 12 |
| 26 | Theoretical Study of the Structural, Energetic, and Electronic Properties of 55-Atom Metal Nanoclusters: A DFT Investigation within van der Waals Corrections, Spinâ€“Orbit Coupling, and PBE+U of 42 Metal Systems. Journal of Physical Chemistry C, 2016, 120, 28844-28856. | 1.5 | 75 |
| 27 | Lattice thermal expansion and anisotropic displacements in ?-sulfur from diffraction experiments and first-principles theory. Journal of Chemical Physics, 2016, 145, 234512. | 1.2 | 19 |
| 28 | Accurate dissociation energies of two isomers of the 1-naphtholâ‹…cyclopropane complex. Journal of Chemical Physics, 2016, 145, 164304. | 1.2 | 19 |
| 29 | Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections. Journal of Chemical Physics, 2016, 145, 204101. | 1.2 | 26 |
| 30 | Dispersion Forces, Disproportionation, and Stable Highâ€Valent Late Transition Metal Alkyls. Angewandte Chemie, 2016, 128, 14986-14989. | 1.6 | 13 |
| 31 | Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. Journal of Chemical Physics, 2016, 145, 044109. | 1.2 | 16 |
| 32 | The structure of water at a Pt(111) electrode and the potential of zero charge studied from first principles. Journal of Chemical Physics, 2016, 144, 194701. | 1.2 | 127 |
| 33 | From single molecules to water networks: Dynamics of water adsorption on Pt(111). Journal of Chemical Physics, 2016, 145, 094703. | 1.2 | 18 |
| 34 | Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 2197-2203. | 2.1 | 305 |
| 35 | Screened exchange hybrid density functional for accurate and efficient structures and interaction energies. Physical Chemistry Chemical Physics, 2016, 18, 15519-15523. | 1.3 | 49 |
| 36 | Organic crystal polymorphism: a benchmark for dispersion-corrected mean-field electronic structure methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 502-513. | 0.5 | 53 |
| 37 | Ïƒâ€Bond Activation in Aluminiumâ€Functionalized Alkynylchlorogermanes: Facile Insertion of Isocyanate and Azide into Alâ€“C and Geâ€“Cl Bonds. European Journal of Inorganic Chemistry, 2016, 2016, 4170-4178. | 1.0 | 6 |
| 38 | Structural, Electronic, and Optical Properties of Bulk Boric Acid 2A and 3T Polymorphs: Experiment and Density Functional Theory Calculations. Crystal Growth and Design, 2016, 16, 6631-6640. | 1.4 | 13 |
| 39 | Systematic and Automated Development of Quantum Mechanically Derived Force Fields: The Challenging Case of Halogenated Hydrocarbons. Journal of Chemical Theory and Computation, 2016, 12, 5525-5540. | 2.3 | 35 |

| # | Article | IF | Citations |
|---|---|---|---|
| 40 | Assessing Ionâ€“Water Interactions in the AMOEBA Force Field Using Energy Decomposition Analysis of Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5422-5437. | 2.3 | 79 |
| 41 | Rotational Barriers of Substituted BIPHEP Ligands: A Comparative Experimental and Theoretical Study. European Journal of Organic Chemistry, 2016, 2016, 5123-5126. | 1.2 | 8 |
| 42 | Accurate adsorption energies for small molecules on oxide surfaces: CH<sub>4</sub>/MgO(001) and C<sub>2</sub>H<sub>6</sub>/MgO(001). Journal of Computational Chemistry, 2016, 37, 2374-2385. | 1.5 | 20 |
| 43 | Dispersion and Hydrogen Bonding Rule: Why the Vaporization Enthalpies of Aprotic Ionic Liquids Are Significantly Larger than those of Protic Ionic liquids. Angewandte Chemie - International Edition, 2016, 55, 11682-11686. | 7.2 | 50 |
| 44 | Why metalâ€“oxos react with dihydroanthracene and cyclohexadiene at comparable rates, despite having different Câ€“H bond strengths. A computational study. Chemical Communications, 2016, 52, 10509-10512. | 2.2 | 28 |
| 45 | The INV24 test set: how well do quantum-chemical methods describe inversion and racemization barriers?. Canadian Journal of Chemistry, 2016, 94, 1133-1143. | 0.6 | 45 |
| 46 | Noncovalent interactions between the second coordination sphere and the active site of [NiFeSe] hydrogenase. RSC Advances, 2016, 6, 81636-81646. | 1.7 | 1 |
| 47 | Understanding the Shape of GeTe Nanocrystals from First Principles. Chemistry of Materials, 2016, 28, 6682-6688. | 3.2 | 16 |
| 48 | Theoretical Study of Cyclic Pyrene Oligomers and Their Resemblance with Cyclic Paraphenylenes: Disclosing Structureâ€“Property Relationships for Cyclic Nanorings. Journal of Physical Chemistry C, 2016, 120, 22069-22078. | 1.5 | 4 |
| 49 | Effect of Li Adsorption on the Electronic and Hydrogen Storage Properties of Acenes: A Dispersion-Corrected TAO-DFT Study. Scientific Reports, 2016, 6, 33081. | 1.6 | 46 |
| 50 | Dispersion Forces, Disproportionation, and Stable Highâ€Valent Late Transition Metal Alkyls. Angewandte Chemie - International Edition, 2016, 55, 14766-14769. | 7.2 | 43 |
| 51 | Alchemical screening of ionic crystals. Physical Chemistry Chemical Physics, 2016, 18, 31078-31091. | 1.3 | 25 |
| 52 | Benchmarking DFT-GGA calculations for the structure optimisation of neutral-framework zeotypes. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 38 |
| 53 | Effect of metal complexation on the equilibrium between methylphosphepine and methylphosphanorcaradiene and their benzo analogues. New Journal of Chemistry, 2016, 40, 7804-7813. | 1.4 | 0 |
| 54 | Benchmark tests of a strongly constrained semilocal functional with a long-range dispersion correction. Physical Review B, 2016, 94, . | 1.1 | 152 |
| 55 | Theoretical Determination of Interaction and Cohesive Energies of Weakly Bound Cycloparaphenylene Molecules. Journal of Physical Chemistry C, 2016, 120, 22627-22634. | 1.5 | 17 |
| 56 | Toward Accurate Adsorption Energetics on Clay Surfaces. Journal of Physical Chemistry C, 2016, 120, 26402-26413. | 1.5 | 30 |
| 57 | Dispersion und WasserstoffbrÃ¼cken bestimmend â€“ Warum die Verdampfungsenthalpien von aprotischen grÃ¶ÃŸer als die von protischen ionischen FlÃ¼ssigkeiten sind. Angewandte Chemie, 2016, 128, 11856-11860. | 1.6 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 58 | van der Waals potential energy surfaces from the exchange-hole dipole moment dispersion model. Canadian Journal of Chemistry, 2016, 94, 1049-1056. | 0.6 | 1 |
| 59 | Assessment of Different Quantum Mechanical Methods for the Prediction of Structure and Cohesive Energy of Molecular Crystals. Journal of Chemical Theory and Computation, 2016, 12, 3340-3352. | 2.3 | 85 |
| 60 | Methane adsorption on the surface of a model of shale: A density functional theory study. Applied Surface Science, 2016, 387, 379-384. | 3.1 | 25 |
| 61 | Benchmark Calculations of Interaction Energies in Noncovalent Complexes and Their Applications. Chemical Reviews, 2016, 116, 5038-5071. | 23.0 | 346 |
| 62 | Towards full Quantumâ€Mechanicsâ€based Proteinâ€“Ligand Binding Affinities. ChemPhysChem, 2017, 18, 898-905. | 1.0 | 46 |
| 63 | Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754. | 23.0 | 181 |
| 64 | Evaluation of DFT-D3 dispersion corrections for various structural benchmark sets. Journal of Chemical Physics, 2017, 146, 044115. | 1.2 | 23 |
| 65 | The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase. Chemical Physics Letters, 2017, 672, 124-127. | 1.2 | 11 |
| 66 | Adsorption of Organic Molecules to van der Waals Materials: Comparison of Fluorographene and Fluorographite with Graphene and Graphite. Journal of Chemical Theory and Computation, 2017, 13, 1328-1340. | 2.3 | 47 |
| 67 | London dispersion forces in sterically crowded inorganic and organometallic molecules. Nature Reviews Chemistry, 2017, 1, . | 13.8 | 296 |
| 68 | Weak Supramolecular Interactions Governing Parallel and Antiparallel DNA Quadruplexes: Insights from Largeâ€Scale Quantum Mechanics Analysis of Experimentally Derived Models. Chemistry - A European Journal, 2017, 23, 5573-5584. | 1.7 | 9 |
| 69 | Development of New Density Functional Approximations. Annual Review of Physical Chemistry, 2017, 68, 155-182. | 4.8 | 51 |
| 70 | First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758. | 23.0 | 408 |
| 71 | Competition of van der Waals and chemical forces on goldâ€“sulfur surfaces and nanoparticles. Nature Reviews Chemistry, 2017, 1, . | 13.8 | 95 |
| 72 | Partnering dispersion corrections with modern parameter-free double-hybrid density functionals. Physical Chemistry Chemical Physics, 2017, 19, 13481-13487. | 1.3 | 31 |
| 73 | Revealing the Intermolecular Interactions of Asphaltene Dimers by Quantum Chemical Calculations. Energy & Fuels, 2017, 31, 2488-2495. | 2.5 | 59 |
| 74 | CO-Reduction Chemistry: Reaction of a CO-Derived Formylhydridoborate with Carbon Monoxide, with Carbon Dioxide, and with Dihydrogen. Journal of the American Chemical Society, 2017, 139, 6474-6483. | 6.6 | 50 |
| 75 | A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1â€“86). Journal of Chemical Theory and Computation, 2017, 13, 1989-2009. | 2.3 | 1,072 |

| # | Article | IF | Citations |
|---|---|---|---|
| 76 | London Dispersion Enables the Shortest Intermolecular Hydrocarbon HÂ·Â·Â·H Contact. Journal of the American Chemical Society, 2017, 139, 7428-7431. | 6.6 | 126 |
| 77 | SparseMapsâ€"A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. Journal of Chemical Physics, 2017, 146, 174108. | 1.2 | 122 |
| 78 | Câ€"F/Câ€"H Functionalization by Manganese(I) Catalysis: Expedient (Per)Fluoro-Allylations and Alkenylations. ACS Catalysis, 2017, 7, 4209-4213. | 5.5 | 165 |
| 79 | Plane-Wave Density Functional Theory Meets Molecular Crystals: Thermal Ellipsoids and Intermolecular Interactions. Accounts of Chemical Research, 2017, 50, 1231-1239. | 7.6 | 47 |
| 80 | Performance of van der Waals Corrected Functionals for Guest Adsorption in the M<sub>2</sub>(dobdc) Metalâ€"Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151. | 1.1 | 41 |
| 81 | Noble Gas Encapsulated Endohedral Zintl Ions Ng@Pb<sub>12</sub><sup>2â€"</sup> and Ng@Sn<sub>12</sub><sup>2â€"</sup> (Ng = He, Ne, Ar, and Kr): A Theoretical Investigation. Journal of Physical Chemistry C, 2017, 121, 11932-11949. | 1.5 | 16 |
| 82 | The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. Chemistry - A European Journal, 2017, 23, 6150-6164. | 1.7 | 102 |
| 83 | Method Dependence of Proline Ring Flexibility in the Poly-<scp>l</scp>-Proline Type II Polymer. Journal of Chemical Theory and Computation, 2017, 13, 370-379. | 2.3 | 16 |
| 84 | Atom- and Ion-Centered Icosahedral Shaped Subnanometer-Sized Clusters of Molecular Hydrogen. Journal of Physical Chemistry C, 2017, 121, 15036-15048. | 1.5 | 7 |
| 85 | Effect of dispersion corrections on covalent and non-covalent interactions in DFTB calculations. Structural Chemistry, 2017, 28, 1399-1407. | 1.0 | 4 |
| 86 | Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. Chemical Science, 2017, 8, 4926-4940. | 3.7 | 97 |
| 87 | Bâ€"H<sub>b</sub>â‹Ï€ interaction in boraneâ€"graphene complexes: coronene as a case study. New Journal of Chemistry, 2017, 41, 5040-5054. | 1.4 | 14 |
| 88 | Computational Modeling and Simulation of CO<sub>2</sub> Capture by Aqueous Amines. Chemical Reviews, 2017, 117, 9524-9593. | 23.0 | 143 |
| 89 | Full Selectivity Control in Cobalt(III)â€Catalyzed Câ^'H Alkylations by Switching of the Câ^'H Activation Mechanism. Angewandte Chemie, 2017, 129, 10514-10518. | 1.6 | 95 |
| 90 | Full Selectivity Control in Cobalt(III)â€Catalyzed Câ^'H Alkylations by Switching of the Câ^'H Activation Mechanism. Angewandte Chemie - International Edition, 2017, 56, 10378-10382. | 7.2 | 243 |
| 91 | Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals. Molecular Physics, 2017, 115, 2315-2372. | 0.8 | 1,401 |
| 92 | Pancake Bond Orders of a Series of Ï€â€Stacked Triangulene Radicals. Angewandte Chemie - International Edition, 2017, 56, 10188-10191. | 7.2 | 46 |
| 93 | Hydrogen adsorption on MoS<sub>2</sub>-surfaces: a DFT study on preferential sites and the effect of sulfur and hydrogen coverage. Physical Chemistry Chemical Physics, 2017, 19, 16231-16241. | 1.3 | 64 |

| # | Article | IF | Citations |
|---|---|---|---|
| 94 | Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. Journal of Chemical Theory and Computation, 2017, 13, 3136-3152. | 2.3 | 81 |
| 95 | Periodic Dispersion-Corrected Approach for Isolation Spectroscopy of N<sub>2</sub> in an Argon Environment: Clusters, Surfaces, and Matrices. Journal of Physical Chemistry A, 2017, 121, 4093-4102. | 1.1 | 4 |
| 96 | Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 2650-2666. | 2.3 | 8 |
| 97 | A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108. | 1.2 | 35 |
| 98 | Reaction Mechanism of Cu(I)-Mediated Reductive CO<sub>2</sub> Coupling for the Selective Formation of Oxalate: Cooperative CO<sub>2</sub> Reduction To Give Mixed-Valence Cu<sub>2</sub>(CO<sub>2</sub><sup>â€¢â€“</sup>) and Nucleophilic-Like Attack. Inorganic Chemistry, 2017, 56, 6809-6819. | 1.9 | 39 |
| 99 | Can DFT and ab initio methods adequately describe binding energies in strongly interacting C6X6â‹¯C2X Ï€â€“Ï€ complexes?. Chemical Physics, 2017, 493, 12-19. | 0.9 | 7 |
| 100 | Assessment of van der Waals inclusive density functional theory methods for layered electroactive materials. Physical Chemistry Chemical Physics, 2017, 19, 10133-10139. | 1.3 | 43 |
| 101 | How strongly do hydrogen and water molecules stick to carbon nanomaterials?. Journal of Chemical Physics, 2017, 146, . | 1.2 | 38 |
| 102 | Methanol Oxidation on Pt(111) from First-Principles in Heterogeneous and Electrocatalysis. Electrocatalysis, 2017, 8, 577-586. | 1.5 | 26 |
| 103 | Role of exact exchange in thermally-assisted-occupation density functional theory: A proposal of new hybrid schemes. Journal of Chemical Physics, 2017, 146, 044102. | 1.2 | 38 |
| 104 | Manganese(I)â€Catalyzed Dispersionâ€Enabled Cå^'H/Cå^'C Activation. Chemistry - A European Journal, 2017, 23, 5443-5447. | 1.7 | 98 |
| 105 | Trapping Experiments on a Trichlorosilanide Anion: a Key Intermediate of Halogenosilane Chemistry. Inorganic Chemistry, 2017, 56, 8683-8688. | 1.9 | 22 |
| 106 | Why Are Vinyl Cations Sluggish Electrophiles?. Journal of the American Chemical Society, 2017, 139, 1499-1511. | 6.6 | 59 |
| 107 | Anziehung gleich geladener Ionen in ionischen FlÃ¼ssigkeiten: Kontrolle der Bildung kationischer Cluster Ã¼ber die WechselwirkungsstÃrke der Gegenionen. Angewandte Chemie, 2017, 129, 510-514. | 1.6 | 21 |
| 108 | When Like Charged Ions Attract in Ionic Liquids: Controlling the Formation of Cationic Clusters by the Interaction Strength of the Counterions. Angewandte Chemie - International Edition, 2017, 56, 496-500. | 7.2 | 81 |
| 109 | Firstâ€principles modeling of molecular crystals: structures and stabilities, temperature and pressure. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1294. | 6.2 | 141 |
| 110 | A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215. | 1.3 | 1,230 |
| 111 | Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. Inorganic Chemistry, 2017, 56, 12485-12491. | 1.9 | 41 |

| # | Article | IF | Citations |
|---|---|---|---|
| 112 | A Computational Scheme To Evaluate Hamaker Constants of Molecules with Practical Size and Anisotropy. Journal of Chemical Theory and Computation, 2017, 13, 5217-5230. | 2.3 | 16 |
| 113 | Inverting Steric Effects: Using â€œAttractiveâ€•Noncovalent Interactions To Direct Silver-Catalyzed Nitrene Transfer. Journal of the American Chemical Society, 2017, 139, 17376-17386. | 6.6 | 52 |
| 114 | Proton transfer and hydrogen bonding in glycosylation reactions. Journal of Carbohydrate Chemistry, 2017, 36, 59-99. | 0.4 | 20 |
| 115 | Study on the pH Dependence of the Photophysical Properties of a Functionalized Perylene Bisimide and Its Potential Applications as a Fluorescence Lifetime Based pH Probe. Journal of Physical Chemistry C, 2017, 121, 24786-24797. | 1.5 | 19 |
| 116 | Noncovalent interactions underlying binary mixtures of amino acid based ionic liquids: insights from theory. Physical Chemistry Chemical Physics, 2017, 19, 29561-29582. | 1.3 | 1 |
| 117 | MD and QM/MM Study of the Quaternary HutP Homohexamer Complex with mRNA, <scp>l</scp>-Histidine Ligand, and Mg<sup>2+</sup>. Journal of Chemical Theory and Computation, 2017, 13, 5658-5670. | 2.3 | 17 |
| 118 | Sandwiches of N-doped diamondoids and benzenevialone pairâ€“cation and cationâ€“pi interaction: a DFT study. New Journal of Chemistry, 2017, 41, 14420-14430. | 1.4 | 8 |
| 119 | Synthesis, Structure, and Luminescence of Copper(I) Halide Complexes of Chiral Bis(phosphines). Inorganic Chemistry, 2017, 56, 12809-12820. | 1.9 | 37 |
| 120 | Thermal Expansion of Carbamazepine: Systematic Crystallographic Measurements Challenge Quantum Chemical Calculations. Journal of Physical Chemistry Letters, 2017, 8, 4319-4324. | 2.1 | 50 |
| 121 | Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. Annual Reports in Computational Chemistry, 2017, 13, 3-91. | 0.9 | 8 |
| 122 | Paving the Way for the Molecular-Level Design of Adsorbents for Carbon Capture: A Quantum-Chemical Investigation of the Adsorption of CO<sub>2</sub> and N<sub>2</sub> on Pure-Silica Chabazite. Journal of Physical Chemistry C, 2017, 121, 19314-19320. | 1.5 | 7 |
| 123 | Attenuation of London Dispersion in Dichloromethane Solutions. Journal of the American Chemical Society, 2017, 139, 13126-13140. | 6.6 | 93 |
| 124 | Quantum mechanical force fields for condensed phase molecular simulations. Journal of Physics Condensed Matter, 2017, 29, 383002. | 0.7 | 22 |
| 125 | Improved description of the structural and optoelectronic properties of DNA/RNA nucleobase anhydrous crystals: Experiment and dispersion-corrected density functional theory calculations. Physical Review B, 2017, 96, . | 1.1 | 13 |
| 126 | Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. Journal of Chemical Theory and Computation, 2017, 13, 5404-5419. | 2.3 | 16 |
| 127 | The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727. | 1.2 | 82 |
| 128 | Synthesis of Electronâ€Rich, Planarized Silicon(IV) Species and a Theoretical Analysis of Dimerizing Aminosilanes. Chemistry - A European Journal, 2017, 23, 17764-17774. | 1.7 | 16 |
| 129 | General optimization procedure towards the design of a new family of minimal parameter spin-component-scaled double-hybrid density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 26191-26200. | 1.3 | 20 |

| # | Article | IF | Citations |
|---|---|---|---|
| 130 | The nature of three-body interactions in DFT: Exchange and polarization effects. Journal of Chemical Physics, 2017, 147, 084106. | 1.2 | 15 |
| 131 | Anthracenyl polar embedded stationary phases with enhanced aromatic selectivity. Part II: A density functional theory study. Journal of Chromatography A, 2017, 1519, 91-99. | 1.8 | 2 |
| 132 | Mechanisms for C(sp2)â€“Si activation of aryltrimethylsilyl groups in palladium-catalysed couplings. Organic and Biomolecular Chemistry, 2017, 15, 8179-8185. | 1.5 | 5 |
| 133 | Is the R<sub>3</sub>Si Moiety in Metalâ€“Silyl Complexes a Z ligand? Anâ€‰Answer from the Interaction Energy. Chemistry - A European Journal, 2017, 23, 17058-17069. | 1.7 | 25 |
| 134 | Thermochemistry of Racemic and Enantiopure Organic Crystals for Predicting Enantiomer Separation. Crystal Growth and Design, 2017, 17, 4676-4686. | 1.4 | 33 |
| 135 | Pancake Bond Orders of a Series of Ïâ€Stacked Triangulene Radicals. Angewandte Chemie, 2017, 129, 10322-10325. | 1.6 | 8 |
| 136 | Quantitative probing of subtle interactions among H-bonds in alpha hydroxy carboxylic acid complexes. Physical Chemistry Chemical Physics, 2017, 19, 24399-24411. | 1.3 | 6 |
| 137 | A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708. | 1.2 | 53 |
| 138 | Extension of the D3 dispersion coefficient model. Journal of Chemical Physics, 2017, 147, 034112. | 1.2 | 617 |
| 139 | On the hydrogen activation by frustrated Lewis pairs in the solid state: benchmark studies and theoretical insights. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170006. | 1.6 | 8 |
| 140 | Secondary Phosphine Oxide Preligands for Palladiumâ€Catalyzed Câ€“H (Hetero)Arylations: Efficient Access to Pybox Ligands. Advanced Synthesis and Catalysis, 2017, 359, 3137-3141. | 2.1 | 20 |
| 141 | Mild Cobalt(III)â€Catalyzed Allylative Câ^'F/Câ^'H Functionalizations at Room Temperature. Chemistry - A European Journal, 2017, 23, 12145-12148. | 1.7 | 95 |
| 142 | Understanding Noncovalent Interactions of Small Molecules with Carbon Nanotubes. Chemistry - A European Journal, 2017, 23, 12909-12916. | 1.7 | 30 |
| 143 | W4â€17: A diverse and highâ€confidence dataset of atomization energies for benchmarking highâ€level electronic structure methods. Journal of Computational Chemistry, 2017, 38, 2063-2075. | 1.5 | 120 |
| 144 | Accurate DFT-D3 Calculations in a Small Basis Set. Journal of Chemical Theory and Computation, 2017, 13, 3575-3585. | 2.3 | 70 |
| 145 | On Atomsâ€inâ€Molecules Energies from Kohnâ€“Sham Calculations. ChemPhysChem, 2017, 18, 2675-2687. | 1.0 | 29 |
| 146 | Dispersion Interactions and the Stability of Amine Dimers. ChemistryOpen, 2017, 6, 571-584. | 0.9 | 6 |
| 147 | Simple way to apply nonlocal van der Waals functionals within all-electron methods. Physical Review B, 2017, 96, . | 1.1 | 16 |

| # | Article | IF | Citations |
|---|---|---|---|
| 148 | Intramolecular interactions in sterically crowded hydrocarbon molecules. Journal of Computational Chemistry, 2017, 38, 2500-2508. | 1.5 | 17 |
| 149 | Reactions of a Ga/Pâ€Based Frustrated Lewis Pair with HX (X = F â€“ I), Heterocumulenes Râ€“NCY (Y = O, S) and Chalcogensâ€“Adduct Formation and Surprising Stability towards Protolysis. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1016-1029. | 0.6 | 16 |
| 150 | Impact of dispersion forces on the atomic structure of a prototypical network-forming disordered system: The case of liquid GeSe2. Journal of Chemical Physics, 2017, 147, 044504. | 1.2 | 9 |
| 151 | Changing the gap type of solid state boric acid by heating: a dispersion-corrected density functional study of Ì±-, Î²-, and Ì³-metaboric acid polymorphs. New Journal of Chemistry, 2017, 41, 15533-15544. | 1.4 | 4 |
| 152 | Tuning the inter-molecular charge transfer, second-order nonlinear optical and absorption spectra properties of a Ï€-dimer under an external electric field. Physical Chemistry Chemical Physics, 2017, 19, 31958-31964. | 1.3 | 16 |
| 153 | Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. Journal of Chemical Theory and Computation, 2017, 13, 6146-6157. | 2.3 | 40 |
| 154 | Polymer Segments at the Folding Limit: Raman Scattering for the Diglyme Benchmark. ChemPhysChem, 2017, 18, 3570-3575. | 1.0 | 1 |
| 155 | Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory. RSC Advances, 2017, 7, 50496-50507. | 1.7 | 33 |
| 156 | On the structure of the P-iodo-, bromo- and chloro-bis(imino)phosphoranes: A DFT study. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 895-901. | 0.3 | 0 |
| 157 | Effect of Li Termination on the Electronic and Hydrogen Storage Properties of Linear Carbon Chains: A TAO-DFT Study. Scientific Reports, 2017, 7, 4966. | 1.6 | 27 |
| 158 | Dispersion corrections applied to the TCA family of exchange-correlation functionals. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 4 |
| 159 | Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144. | 1.5 | 23 |
| 160 | Controlling the kinetic and thermodynamic stability of cationic clusters by the addition of molecules or counterions. Physical Chemistry Chemical Physics, 2017, 19, 18854-18862. | 1.3 | 29 |
| 161 | Understanding the Role of Dispersion in Frustrated Lewis Pairs and Classical Lewis Adducts: A Domainâ€Based Local Pair Natural Orbital Coupled Cluster Study. Chemistry - A European Journal, 2017, 23, 865-873. | 1.7 | 91 |
| 162 | Cooperative Activation of Isocyanates by Alâ€“Nâ€Based Active Lewis Pairs and the Generation of a C<sub>5</sub> Chain by Simultaneous Formation of Two Câ€“C Bonds. Chemistry - A European Journal, 2017, 23, 6129-6141. | 1.7 | 15 |
| 163 | Sizing the role of London dispersion in the dissociation of all-meta tert-butyl hexaphenylethane. Chemical Science, 2017, 8, 405-410. | 3.7 | 104 |
| 164 | Computational Chemistry Methods for Nanoporous Materials. Chemistry of Materials, 2017, 29, 199-212. | 3.2 | 69 |
| 166 | Noncovalent Interactions in Molecular Crystals. , 2017, , 303-331. | | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 167 | Molecular Crystal Structure Prediction. , 2017, , 333-363. | | 16 |
| 168 | A Comprehensive Overview of the DFT-D3 London-Dispersion Correction. , 2017, , 195-219. | | 57 |
| 169 | Noncovalent Interactions in the Catechol Dimer. Biomimetics, 2017, 2, 18. | 1.5 | 17 |
| 170 | Density Functional Theory Investigation into the B and Ga Doped Clean and Water Covered Î³-Alumina Surfaces. Journal of Chemistry, 2017, 2017, 1-7. | 0.9 | 4 |
| 171 | A First Principles Study of H2 Adsorption on LaNiO3(001) Surfaces. Materials, 2017, 10, 36. | 1.3 | 8 |
| 172 | Benchmarking the performance of density-functional-based approaches on intermolecular interactions of Heliumâ€“water complexes. Journal of Physics: Conference Series, 2017, 875, 102026. | 0.3 | 1 |
| 173 | Intermolecular Interaction Energies from Kohnâ€“Sham Random Phase Approximation Correlation Methods. , 2017, , 65-136. | | 6 |
| 174 | Toward Accurate Conformational Energies of Smaller Peptides and Medium-Sized Macrocycles: MPCONF196 Benchmark Energy Data Set. Journal of Chemical Theory and Computation, 2018, 14, 1254-1266. | 2.3 | 69 |
| 175 | Comment on â€œHYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributionsâ€• Journal of Physical Chemistry B, 2018, 122, 2825-2826. | 1.2 | 4 |
| 176 | Cluster approach to the prediction of thermodynamic and transport properties of ionic liquids. Journal of Chemical Physics, 2018, 148, 193832. | 1.2 | 11 |
| 177 | Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835. | 1.2 | 38 |
| 178 | Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2265-2276. | 2.3 | 18 |
| 179 | Quantumâ€mechanical condensed matter simulations with CRYSTAL. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1360. | 6.2 | 1,277 |
| 180 | Computational prediction of chemical reactions: current status and outlook. Drug Discovery Today, 2018, 23, 1203-1218. | 3.2 | 126 |
| 181 | Importance of van der Waals interaction on structural, vibrational, and thermodynamic properties of NaCl. Solid State Communications, 2018, 273, 11-16. | 0.9 | 16 |
| 182 | in,in-Cyclophanes with Bridgehead Methyl Groups. Organic Letters, 2018, 20, 2576-2579. | 2.4 | 3 |
| 183 | Simplified DFT methods for consistent structures and energies of large systems. Journal of Physics Condensed Matter, 2018, 30, 213001. | 0.7 | 42 |
| 184 | Ab initio prediction of the polymorph phase diagram for crystalline methanol. Chemical Science, 2018, 9, 4622-4629. | 3.7 | 53 |

| # | Article | IF | Citations |
|---|---|---|---|
| 185 | Rotational and translational dynamics and their relation to hydrogen bond lifetimes in an ionic liquid by means of NMR relaxation time experiments and molecular dynamics simulation. Journal of Chemical Physics, 2018, 148, 193843. | 1.2 | 22 |
| 186 | Atomic Orbital Implementation of Extended Symmetry-Adapted Perturbation Theory (XSAPT) and Benchmark Calculations for Large Supramolecular Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2955-2978. | 2.3 | 43 |
| 187 | Quest for Insight into Ultrashort Câ€"HÂ·Â·Â·Ï€ Proximities in Molecular â€œIron Maidensâ€• Journal of Organic Chemistry, 2018, 83, 5114-5122. | 1.7 | 8 |
| 188 | Likeâ€•likesâ€•Like: Cooperative Hydrogen Bonding Overcomes Coulomb Repulsion in Cationic Clusters with Net Charges up to Q =+6 e. ChemPhysChem, 2018, 19, 1691-1695. | 1.0 | 29 |
| 189 | Revealing weak spin-orbit coupling effects on charge carriers in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -conjugated polymer. Physical Review B, 2018, 97, . | 1.1 | 26 |
| 190 | Statistical Analysis of Semiclassical Dispersion Corrections. Journal of Chemical Theory and Computation, 2018, 14, 2480-2494. | 2.3 | 25 |
| 191 | Benchmarking several van der Waals dispersion approaches for the description of intermolecular interactions. Journal of Chemical Physics, 2018, 148, 064112. | 1.2 | 37 |
| 192 | Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. Journal of Chemical Theory and Computation, 2018, 14, 1614-1623. | 2.3 | 164 |
| 193 | Density-Dependent Formulation of Dispersionâ€"Repulsion Interactions in Hybrid Multiscale Quantum/Molecular Mechanics (QM/MM) Models. Journal of Chemical Theory and Computation, 2018, 14, 1671-1681. | 2.3 | 24 |
| 194 | An Exceptionally Close, Nonâ€•Bonded Hydrogenâ€"Hydrogen Contact with Strong Throughâ€•Space Spinâ€"Spin Coupling. Angewandte Chemie, 2018, 130, 2266-2269. | 1.6 | 2 |
| 195 | Supramolecular polymer chemistry meets computational chemistry: theoretical simulations on advanced self-assembling chiral materials. Supramolecular Chemistry, 2018, 30, 876-890. | 1.5 | 3 |
| 196 | The influence of like-charge attraction on the structure and dynamics of ionic liquids: NMR chemical shifts, quadrupole coupling constants, rotational correlation times and failure of Stokesâ€"Einsteinâ€"Debye. Physical Chemistry Chemical Physics, 2018, 20, 5617-5625. | 1.3 | 26 |
| 197 | Introducing DDEC6 atomic population analysis: part 4. Efficient parallel computation of net atomic charges, atomic spin moments, bond orders, and more. RSC Advances, 2018, 8, 2678-2707. | 1.7 | 129 |
| 198 | From Noncovalent Chalcogenâ€"Chalcogen Interactions to Supramolecular Aggregates: Experiments and Calculations. Chemical Reviews, 2018, 118, 2010-2041. | 23.0 | 244 |
| 199 | Fast and accurate quantum Monte Carlo for molecular crystals. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 1724-1729. | 3.3 | 69 |
| 200 | B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104. | 1.2 | 400 |
| 201 | Pushing Electronsâ€"Which Carbene Ligand for Which Application?. Organometallics, 2018, 37, 275-289. | 1.1 | 199 |
| 202 | Application of the Interacting Quantum Atoms Approach to the S66 and Ionicâ€•Hydrogenâ€•Bond Datasets for Noncovalent Interactions. ChemPhysChem, 2018, 19, 973-987. | 1.0 | 21 |

| # | Article | IF | Citations |
|---|---|---|---|
| 203 | Hydrogen bonding in protic ionic liquids: structural correlations, vibrational spectroscopy, and rotational dynamics of liquid ethylammonium nitrate. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 034002. | 0.6 | 21 |
| 204 | Enantioselectivity in CPA-catalyzed Friedelâ€“Crafts reaction of indole and N-tosylimines: a challenge for guiding models. Organic and Biomolecular Chemistry, 2018, 16, 2225-2238. | 1.5 | 11 |
| 205 | Citronellal assumes a folded conformation in solution due to dispersion interactions: A joint NMR-DFT analysis. Journal of Molecular Structure, 2018, 1157, 401-407. | 1.8 | 5 |
| 206 | Conductance Switching in Expanded Porphyrins through Aromaticity and Topology Changes. Journal of the American Chemical Society, 2018, 140, 1313-1326. | 6.6 | 56 |
| 207 | An Exceptionally Close, Nonâ€Bonded Hydrogenâ€“Hydrogen Contact with Strong Throughâ€Space Spinâ€“Spin Coupling. Angewandte Chemie - International Edition, 2018, 57, 2244-2247. | 7.2 | 20 |
| 208 | Vibrational Properties of Bulk Boric Acid2Aand3TPolymorphs and Their Two-Dimensional Layers: Measurements and Density Functional Theory Calculations. Journal of Physical Chemistry A, 2018, 122, 1312-1325. | 1.1 | 10 |
| 209 | Aurophilic Interactions in [(L)AuCl]...[(Lâ€²)AuCl] Dimers: Calibration by Experiment and Theory. Journal of the American Chemical Society, 2018, 140, 2316-2325. | 6.6 | 48 |
| 210 | Accurate geometries for â€œMountain passâ€•regions of the Ramachandran plot using quantum chemical calculations. Proteins: Structure, Function and Bioinformatics, 2018, 86, 273-278. | 1.5 | 7 |
| 211 | How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. Journal of Physical Chemistry Letters, 2018, 9, 464-470. | 2.1 | 22 |
| 212 | Comparison of the Performance of van der Waals Dispersion Functionals in the Description of Water and Ethanol on Transition Metal Surfaces. Journal of Physical Chemistry C, 2018, 122, 1577-1588. | 1.5 | 36 |
| 213 | Interaction Energy Landscapes of Aromatic Heterocycles through a Reliable yet Affordable Computational Approach. Journal of Chemical Theory and Computation, 2018, 14, 543-556. | 2.3 | 23 |
| 214 | Structure and Stability of Molecular Crystals with Many-Body Dispersion-Inclusive Density Functional Tight Binding. Journal of Physical Chemistry Letters, 2018, 9, 399-405. | 2.1 | 37 |
| 215 | Highâ€Level Ab Initio Calculations of Intermolecular Interactions: Heavy Mainâ€Group Element Ï€â€Interactions. Chemistry - A European Journal, 2018, 24, 10238-10245. | 1.7 | 22 |
| 216 | Crystalline Moduli of Polymers, Evaluated from Density Functional Theory Calculations under Periodic Boundary Conditions. ACS Omega, 2018, 3, 4824-4835. | 1.6 | 24 |
| 217 | Estimations of energy of noncovalent bonding from integrals over interatomic zeroâ€flux surfaces: Correlation trends and beyond. Journal of Computational Chemistry, 2018, 39, 1607-1616. | 1.5 | 34 |
| 218 | Intermolecular dissociation energies of dispersively bound complexes of aromatics with noble gases and nitrogen. Journal of Chemical Physics, 2018, 148, 134302. | 1.2 | 21 |
| 219 | An accurate empirical method to predict the adsorption strength for Ï€-orbital contained molecules on two dimensional materials. Journal of Molecular Graphics and Modelling, 2018, 82, 93-100. | 1.3 | 25 |
| 220 | Identifying pragmatic quasi-harmonic electronic structure approaches for modeling molecular crystal thermal expansion. Faraday Discussions, 2018, 211, 181-207. | 1.6 | 29 |

| # | Article | IF | Citations |
|---|---|---|---|
| 221 | Lowest-Energy Crystalline Polymorphs of P3HT. Journal of Physical Chemistry C, 2018, 122, 9141-9151. | 1.5 | 18 |
| 222 | Understanding titanium-catalysed radicalâ€“radical reactions: a DFT study unravels the complex kinetics of ketoneâ€“nitrile couplings. Dalton Transactions, 2018, 47, 5072-5082. | 1.6 | 18 |
| 223 | Rocksalt or cesium chloride: Investigating the relative stability of the cesium halide structures with random phase approximation based methods. Physical Review B, 2018, 97, . | 1.1 | 13 |
| 224 | Crystal structure prediction of flexible pharmaceutical-like molecules: density functional tight-binding as an intermediate optimisation method and for free energy estimation. Faraday Discussions, 2018, 211, 275-296. | 1.6 | 29 |
| 225 | Software update: the ORCA program system, version 4.0. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1327. | 6.2 | 3,771 |
| 226 | A first-principles study on Pd modified ZSM-12 zeolites. Microporous and Mesoporous Materials, 2018, 260, 227-234. | 2.2 | 10 |
| 227 | Trivalent ions modification for high-silica mordenite: A first principles study. Applied Surface Science, 2018, 433, 627-638. | 3.1 | 15 |
| 228 | Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€. ACS Catalysis, 2018, 8, 1371-1375. | 5.5 | 17 |
| 229 | Graphene Oxide Epoxy (GOâ€xy): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities. Advanced Materials Interfaces, 2018, 5, 1700657. | 1.9 | 19 |
| 230 | Organocatalytic Enantioselective Higherâ€Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. Angewandte Chemie - International Edition, 2018, 57, 1246-1250. | 7.2 | 42 |
| 231 | Crystalline packing in pentacene-like organic semiconductors. CrystEngComm, 2018, 20, 63-74. | 1.3 | 59 |
| 232 | Computerchemie: das Schicksal aktueller Methoden und zukÃ¼nftige Herausforderungen. Angewandte Chemie, 2018, 130, 4241-4248. | 1.6 | 16 |
| 233 | Computational Chemistry: The Fate of Current Methods and Future Challenges. Angewandte Chemie - International Edition, 2018, 57, 4170-4176. | 7.2 | 138 |
| 234 | O<sub>2</sub> Activation by Metal Surfaces: Implications for Bonding and Reactivity on Heterogeneous Catalysts. Chemical Reviews, 2018, 118, 2816-2862. | 23.0 | 363 |
| 235 | Distal Weak Coordination of Acetamides in Ruthenium(II)â€Catalyzed Câ^'H Activation Processes. Angewandte Chemie, 2018, 130, 773-776. | 1.6 | 22 |
| 236 | Distal Weak Coordination of Acetamides in Ruthenium(II)â€Catalyzed Câ^'H Activation Processes. Angewandte Chemie - International Edition, 2018, 57, 765-768. | 7.2 | 83 |
| 237 | Bareversusprotected tetrairidium clusters by density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 29480-29492. | 1.3 | 4 |
| 238 | Molecular interactions in electron-groups embedding generalized valence bond picture. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 239 | Quantum-chemical modelling of clay mineral surfaces and clay mineralâ€“surfaceâ€“adsorbate interactions. Developments in Clay Science, 2018, 9, 49-87. | 0.3 | 7 |
| 240 | Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein Journal of Organic Chemistry, 2018, 14, 1181-1191. | 1.3 | 15 |
| 241 | Quantitative Chiral Analysis by Molecular Rotational Spectroscopy. , 2018, , 679-729. | | 35 |
| 242 | Experimental and Computational Evidence for â€œDouble Pancake Bondsâ€• The Role of Dispersion-Corrected DFT Methods in Strongly Dimerized 5-Aryl-1Î»<sup>2</sup>,3Î»<sup>2</sup>-dithia-2,4,6-triazines. ACS Omega, 2018, 3, 18170-18180. | 1.6 | 8 |
| 243 | Stacking Principles on Ï€- and Lamellar Stacking for Organic Semiconductors Evaluated by Energy Decomposition Analysis. ACS Omega, 2018, 3, 18656-18662. | 1.6 | 29 |
| 244 | Low-scaling analytical gradients for the direct random phase approximation using an atomic orbital formalism. Journal of Chemical Physics, 2018, 149, 244111. | 1.2 | 16 |
| 245 | Dependence of the multipole moments, static polarizabilities, and static hyperpolarizabilities of the hydrogen molecule on the Hâ€“H separation in the ground singlet state. Journal of Chemical Physics, 2018, 149, 234103. | 1.2 | 9 |
| 246 | Spektroskopischer Nachweis einer attraktiven Kationâ€Kationâ€Wechselwirkung in OHâ€funktionalisierten ionischen FlÃ¼ssigkeiten: ein Hâ€BrÃ¼ckenâ€gebundenes kettenfÃ¶rmiges Trimer. Angewandte Chemie, 2018, 130, 15590-15594. | 1.6 | 9 |
| 247 | Adsorption of PTCDA on NaCl Surfaces with Color Centers: Charge Transfer and Formation of Radical Ions. Journal of Physical Chemistry C, 2018, 122, 29426-29434. | 1.5 | 7 |
| 248 | Impact of Lowâ€Frequency Vibrations on Charge Transport in Highâ€Mobility Organic Semiconductors. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800485. | 1.2 | 11 |
| 249 | Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective. Batteries, 2018, 4, 62. | 2.1 | 36 |
| 250 | Intermolecular dissociation energies of hydrogen-bonded 1-naphthol complexes. Journal of Chemical Physics, 2018, 149, 204311. | 1.2 | 8 |
| 251 | Performance of Density-Functional Tight-Binding in Comparison to Ab Initio and First-Principles Methods for Isomer Geometries and Energies of Glucose Epimers in Vacuo and Solution. ACS Omega, 2018, 3, 16899-16915. | 1.6 | 12 |
| 252 | Self-Assembly of Nanocubic Molecular Capsules via Solvent-Guided Formation of Rectangular Blocks. Journal of Physical Chemistry Letters, 2018, 9, 6082-6088. | 2.1 | 5 |
| 253 | A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). Journal of Chemical Theory and Computation, 2018, 14, 5128-5142. | 2.3 | 19 |
| 254 | Spectroscopic Evidence for an Attractive Cationâ€“Cation Interaction in Hydroxyâ€Functionalized Ionic Liquids: A Hydrogenâ€Bonded Chainâ€like Trimer. Angewandte Chemie - International Edition, 2018, 57, 15364-15368. | 7.2 | 51 |
| 255 | Constructing soft-conjugated materials from small molecules to polymers: a theoretical study. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 1 |
| 256 | The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and Ï‰B97M-V Approaches. Journal of Chemical Theory and Computation, 2018, 14, 5725-5738. | 2.3 | 170 |

| # | Article | IF | Citations |
|---|---|---|---|
| 257 | Cationic clustering influences the phase behaviour of ionic liquids. Scientific Reports, 2018, 8, 14753. | 1.6 | 51 |
| 258 | Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435. | 1.0 | 5 |
| 259 | The Shape of Native Plant Cellulose Microfibrils. Scientific Reports, 2018, 8, 13983. | 1.6 | 86 |
| 260 | Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381. | 1.6 | 7 |
| 261 | Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. International Journal of Quantum Chemistry, 2018, 118, e25799. | 1.0 | 46 |
| 262 | Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 5715-5724. | 2.3 | 9 |
| 263 | A selenium-catalysed para-amination of phenols. Nature Communications, 2018, 9, 4293. | 5.8 | 43 |
| 264 | Assessment of a range-separated orbital-optimised random-phase approximation electron correlation method. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 6 |
| 265 | Dispersion Energy of Symmetry-Adapted Perturbation Theory from the Explicitly Correlated F12 Approach. Journal of Chemical Theory and Computation, 2018, 14, 5105-5117. | 2.3 | 9 |
| 266 | Vibrational Modes and Phonon and Thermodynamic Properties of the Metaboric Acid Polymorphs Î±-, Î²-, and Î³-(BOH)<sub>3</sub>O<sub>3</sub> within a Density Functional Theory Framework. Journal of Physical Chemistry A, 2018, 122, 7628-7645. | 1.1 | 4 |
| 267 | Highly-sensitive optical organic vapor sensor through polymeric swelling induced variation of fluorescent intensity. Nature Communications, 2018, 9, 3799. | 5.8 | 86 |
| 268 | Reduktion von Phosphanoxiden mit Oxalylchlorid und Wasserstoff, vermittelt durch ein elektrophiles Phosphoniumkation. Angewandte Chemie, 2018, 130, 15473-15476. | 1.6 | 7 |
| 269 | Electrophilic Phosphonium Cationâ€Mediated Phosphane Oxide Reduction Using Oxalyl Chloride and Hydrogen. Angewandte Chemie - International Edition, 2018, 57, 15253-15256. | 7.2 | 37 |
| 270 | Accurate lattice geometrical parameters and bulk moduli from a semilocal density functional. AIP Advances, 2018, 8, . | 0.6 | 15 |
| 271 | QM/MM Calculations on Proteinâ€“RNA Complexes: Understanding Limitations of Classical MD Simulations and Search for Reliable Cost-Effective QM Methods. Journal of Chemical Theory and Computation, 2018, 14, 5419-5433. | 2.3 | 34 |
| 272 | DFT calculations of solids in the ground state. , 2018, , 67-100. | | 2 |
| 273 | Dinuclear Tricyclic Transition State Model for Carbonyl Addition of Organotitanium Reagents: DFT Study on the Activity and Enantioselectivity of BINOLate Titanium Catalysts. Journal of Organic Chemistry, 2018, 83, 7825-7835. | 1.7 | 1 |
| 274 | Effects of Dispersion Corrections and Nonlocality on Density Functional Predictions of Pressure-Induced Polymorphic Transitions of Crystalline Diborane. Journal of Physical Chemistry C, 2018, 122, 14781-14787. | 1.5 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 275 | Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. Journal of Chemical Theory and Computation, 2018, 14, 3004-3013. | 2.3 | 27 |
| 276 | Structural Motifs in Cold Ternary Ion Complexes of Hydroxyl-Functionalized Ionic Liquids: Isolating the Role of Cationâ€“Cation Interactions. Journal of Physical Chemistry Letters, 2018, 9, 2979-2984. | 2.1 | 47 |
| 277 | Sweet graphene: exfoliation of graphite and preparation of glucose-graphene cocrystals through mechanochemical treatments. Green Chemistry, 2018, 20, 3581-3592. | 4.6 | 56 |
| 278 | Density-functional tight-binding approach for metal clusters, nanoparticles, surfaces and bulk: application to silver and gold. Journal of Physics Condensed Matter, 2018, 30, 303001. | 0.7 | 24 |
| 279 | First-principles stability ranking of molecular crystal polymorphs with the DFT+MBD approach. Faraday Discussions, 2018, 211, 253-274. | 1.6 | 39 |
| 280 | Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. Physical Chemistry Chemical Physics, 2018, 20, 23175-23194. | 1.3 | 102 |
| 281 | Development and Validation of Quantum Mechanically Derived Force-Fields: Thermodynamic, Structural, and Vibrational Properties of Aromatic Heterocycles. Journal of Chemical Theory and Computation, 2018, 14, 4884-4900. | 2.3 | 26 |
| 282 | Unraveling substituent effects on the glass transition temperatures of biorenewable polyesters. Nature Communications, 2018, 9, 2880. | 5.8 | 58 |
| 283 | Geometry optimisations with a nonlocal density-functional theory method based on a double Hirshfeld partitioning. Journal of Chemical Physics, 2018, 149, 044103. | 1.2 | 2 |
| 284 | Intermolecular dissociation energies of 1-naphtholÂ·n-alkane complexes. Journal of Chemical Physics, 2018, 149, 034306. | 1.2 | 7 |
| 285 | Communication: Accurate description of interaction energies and three-body effects in weakly bound molecular complexes by PBE-QIDH models. Journal of Chemical Physics, 2018, 149, 041101. | 1.2 | 4 |
| 286 | On the exfoliation and anisotropic thermal expansion of black phosphorus. Chemical Communications, 2018, 54, 9793-9796. | 2.2 | 15 |
| 287 | Attractive Nonbonded Interactions Help Stabilize the Z Form of Alkenyl Anions. Journal of Organic Chemistry, 2018, 83, 8208-8213. | 1.7 | 4 |
| 288 | Mutual Kinetic Resolution of Racemic 3,4â€Dihydroâ€3â€methylâ€2Hâ€[1,4]benzoxazines with Acyl Chlorides of Racemic Oâ€Phenyllactic Acids and DFT Modelling of Transition States. European Journal of Organic Chemistry, 2018, 2018, 4577-4585. | 1.2 | 11 |
| 289 | Toward a Reliable Description of the Lattice Vibrations in Organic Molecular Crystals: The Impact of van der Waals Interactions. Journal of Chemical Theory and Computation, 2018, 14, 4380-4390. | 2.3 | 26 |
| 290 | Quantum chemical exploration of formaldehyde clusters (H<sub>2</sub>CO)<sub>n</sub> (nâ€‰=â€‰2â€“4). Journal of Computational Chemistry, 2018, 39, 1498-1507. | 1.5 | 11 |
| 292 | The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit. Australian Journal of Chemistry, 2018, 71, 238. | 0.5 | 40 |
| 293 | Bâ‹¯H<sub>b</sub>â†X (X= N, O, P, S, F, Cl, Br) interactions: A density functional study. International Journal of Quantum Chemistry, 2018, 118, e25654. | 1.0 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 294 | Exposing Key Vibrational Contributions to Properties of Organic Molecular Solids with High Signal, Low Frequency Neutron Spectroscopy and Ab Initio Simulations. Crystal Growth and Design, 2018, 18, 4815-4821. | 1.4 | 5 |
| 295 | Superbenzeneâ€“Porphyrin Gasâ€Phase Architectures Derived from Intermolecular Dispersion Interactions. Chemistry - A European Journal, 2018, 24, 15818-15824. | 1.7 | 21 |
| 296 | Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. Methods in Enzymology, 2018, 607, 53-90. | 0.4 | 11 |
| 297 | The electric double layer at metal-water interfaces revisited based on a charge polarization scheme. Journal of Chemical Physics, 2018, 149, 084705. | 1.2 | 128 |
| 298 | Quantum-Chemical Insights into the Self-Assembly of Carbon-Based Supramolecular Complexes. Molecules, 2018, 23, 118. | 1.7 | 9 |
| 299 | Accurate Noncovalent Interactions via Dispersion-Corrected Second-Order MÃllerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2018, 14, 4711-4721. | 2.3 | 41 |
| 300 | Short is strong: experimental electron density in a very short NÂ·Â·Â·I halogen bond. Zeitschrift Fur Kristallographie - Crystalline Materials, 2018, 233, 733-744. | 0.4 | 17 |
| 301 | Evaluation of dispersion type metalÂ·Â·Â·Ï€ arene interaction in arylbismuth compounds â€“ an experimental and theoretical study. Beilstein Journal of Organic Chemistry, 2018, 14, 2125-2145. | 1.3 | 25 |
| 302 | A spectroscopic study of indigo dye in aqueous solution: A combined experimental and TD-DFT study. Journal of Luminescence, 2018, 204, 568-572. | 1.5 | 3 |
| 303 | A Systematic Protocol for Benchmarking Guestâ€“Host Interactions by Firstâ€Principles Computations: Capturing CO<sub>2</sub> in Clathrate Hydrates. Chemistry - A European Journal, 2018, 24, 9353-9363. | 1.7 | 13 |
| 304 | Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2018, 14, 3524-3531. | 2.3 | 37 |
| 305 | Survival of the most transferable at the top of Jacobâ€™s ladder: Defining and testing the Ï‰B97M(2) double hybrid density functional. Journal of Chemical Physics, 2018, 148, 241736. | 1.2 | 136 |
| 306 | Stimulating intra- and intermolecular charge transfer and nonlinear optical response for biphenalenyl biradicaloid dimer under an external electric field. Physical Chemistry Chemical Physics, 2018, 20, 18699-18706. | 1.3 | 14 |
| 307 | Pancake Bonding: An Unusual Piâ€Stacking Interaction. Chemistry - A European Journal, 2019, 25, 400-416. | 1.7 | 171 |
| 308 | Noncovalent interactions in inorganic supramolecular chemistry based in heavy metals. Quantum chemistry point of view. International Journal of Quantum Chemistry, 2019, 119, e25675. | 1.0 | 27 |
| 309 | Vacuum-Level Shift at Al/LiF/Alq<sub>3</sub> Interfaces: A First-Principles Study. ACS Omega, 2019, 4, 13426-13434. | 1.6 | 3 |
| 310 | Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Waterâ€“Air Interface. Journal of Physical Chemistry Letters, 2019, 10, 4914-4919. | 2.1 | 43 |
| 311 | A comparison of computational methodologies for the structural modelling of biologically relevant zinc complexes. Journal of Molecular Modeling, 2019, 25, 258. | 0.8 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 312 | How to Model Inter- and Intramolecular Hydrogen Bond Strengths with Quantum Chemistry. Journal of Chemical Information and Modeling, 2019, 59, 3735-3743. | 2.5 | 7 |
| 313 | Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 8481-8502. | 5.5 | 75 |
| 314 | Evolutionary Algorithmâ€Based Crystal Structure Prediction for Copper(I) Fluoride. Chemistry - A European Journal, 2019, 25, 11528-11537. | 1.7 | 6 |
| 315 | Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. Angewandte Chemie - International Edition, 2019, 58, 14281-14288. | 7.2 | 24 |
| 316 | Compensation of London Dispersion in the Gas Phase and in Aprotic Solvents. Angewandte Chemie, 2019, 131, 14419-14426. | 1.6 | 4 |
| 317 | Off-the-shelf DFT-DISPersion methods: Are they now â€œon-trendâ€•for organic molecular crystals?. Journal of Chemical Physics, 2019, 151, 044106. | 1.2 | 11 |
| 318 | Nonclassical Bâ€H b â‹¯Ï€ interaction in diboraneâ‹¯localizedâ€Ï€ sandwiches: A DFTâ€D3 study. International Journal of Quantum Chemistry, 2019, 119, e25998. | 1.0 | 2 |
| 319 | Stereoinversion in the diastereoselective acylation of benzoxazine derivatives with 2-aryloxypropionyl chlorides. Russian Chemical Bulletin, 2019, 68, 1257-1263. | 0.4 | 5 |
| 320 | Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constantsâ€”Comparison with Salt Bridges and Molecular Systems. Angewandte Chemie, 2019, 131, 18027-18035. | 1.6 | 7 |
| 321 | Hydrogen Bonding Between Ions of Like Charge in Ionic Liquids Characterized by NMR Deuteron Quadrupole Coupling Constantsâ€”Comparison with Salt Bridges and Molecular Systems. Angewandte Chemie - International Edition, 2019, 58, 17863-17871. | 7.2 | 41 |
| 322 | CrystaLattE: Automated computation of lattice energies of organic crystals exploiting the many-body expansion to achieve dual-level parallelism. Journal of Chemical Physics, 2019, 151, 144103. | 1.2 | 14 |
| 323 | Theoretical studies on the bond strength and electron density characteristics in multiple hydrogen bonded arrays. Journal of Molecular Graphics and Modelling, 2019, 93, 107439. | 1.3 | 10 |
| 324 | Chiral Self Recognition: Interactions in Propylene Oxide Complexes. Journal of Physical Chemistry A, 2019, 123, 8607-8618. | 1.1 | 4 |
| 325 | Fantasy versus reality in fragment-based quantum chemistry. Journal of Chemical Physics, 2019, 151, 170901. | 1.2 | 102 |
| 326 | Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 29556-29570. | 1.5 | 22 |
| 327 | Evaluierung von Londonâ€Dispersionsâ€•und LÃ¶sungsmittelâ€Interaktionen an Alkylâ€Alkylâ€Grenzflächen mittels Azobenzolschaltern. Angewandte Chemie, 2019, 131, 18724-18729. | 1.6 | 12 |
| 328 | Exploring London Dispersion and Solvent Interactions at Alkylâ€“Alkyl Interfaces Using Azobenzene Switches. Angewandte Chemie - International Edition, 2019, 58, 18552-18556. | 7.2 | 45 |
| 329 | Gaussian Process-Based Refinement of Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 6046-6060. | 2.3 | 44 |

| # | Article | IF | Citations |
|---|---|---|---|
| 330 | How much do we know about seabird bycatch in pelagic longline fisheries? A simulation study on the potential bias caused by the usually unobserved portion of seabird bycatch. PLoS ONE, 2019, 14, e0220797. | 1.1 | 5 |
| 331 | Exploring Chemical Bonding in Phaseâ€Change Materials with Orbitalâ€Based Indicators. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800579. | 1.2 | 22 |
| 332 | Interaction between water and carbon nanostructures: How good are current density functional approximations?. Journal of Chemical Physics, 2019, 151, 164702. | 1.2 | 47 |
| 333 | Long-range dispersion-corrected density functional for noncovalent interactions. International Journal of Modern Physics B, 2019, 33, 1950300. | 1.0 | 5 |
| 334 | Isotropic Site-Site Dispersion Potential Determined from Localized Frequency-Dependent Density Susceptibility. Bulletin of the Chemical Society of Japan, 2019, 92, 1694-1700. | 2.0 | 3 |
| 335 | A Linear-Scaling Method for Noncovalent Interactions: An Efficient Combination of Absolutely Localized Molecular Orbitals and a Local Random Phase Approximation Approach. Journal of Chemical Theory and Computation, 2019, 15, 5352-5369. | 2.3 | 4 |
| 336 | Platinum, gold, and silver standards of intermolecular interaction energy calculations. Journal of Chemical Physics, 2019, 151, 070901. | 1.2 | 33 |
| 337 | A noncovalent interaction insight onto the concerted metallation deprotonation mechanism. Physical Chemistry Chemical Physics, 2019, 21, 20486-20498. | 1.3 | 17 |
| 338 | Density Functional Calculations for Aqueous Silver Clusters Containing Water and Nitrate Ligands. Journal of Physical Chemistry B, 2019, 123, 8300-8312. | 1.2 | 0 |
| 339 | HFLD: A Nonempirical London Dispersion-Corrected Hartreeâ€“Fock Method for the Quantification and Analysis of Noncovalent Interaction Energies of Large Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 5894-5907. | 2.3 | 36 |
| 340 | Revisiting the Potential Energy Surface of the Stacked Cytosine Dimer: FNO-CCSD(T) Interaction Energies, SAPT Decompositions, and Benchmarking. Journal of Physical Chemistry A, 2019, 123, 9209-9222. | 1.1 | 9 |
| 341 | Cost-Effective Quantum Mechanical Approach for Predicting Thermodynamic and Mechanical Stability of Pure-Silica Zeolites. ACS Omega, 2019, 4, 1838-1846. | 1.6 | 17 |
| 342 | Adjusting dispersion parameters for the density-functional tight-binding description of molecular crystals. Chemical Physics Letters, 2019, 718, 7-11. | 1.2 | 5 |
| 343 | Origin of the Immiscibility of Alkanes and Perfluoroalkanes. Journal of the American Chemical Society, 2019, 141, 3489-3506. | 6.6 | 45 |
| 344 | Adhesion, forces and the stability of interfaces. Beilstein Journal of Organic Chemistry, 2019, 15, 106-129. | 1.3 | 3 |
| 345 | The interaction of aluminum with catecholamine-based neurotransmitters: can the formation of these species be considered a potential risk factor for neurodegenerative diseases?. Dalton Transactions, 2019, 48, 6003-6018. | 1.6 | 16 |
| 346 | TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between (C<sub>5</sub>Ph<sub>5</sub>)Cr(CO)<sub>3</sub>H and a Trityl Radical. Journal of the American Chemical Society, 2019, 141, 1882-1886. | 6.6 | 25 |
| 347 | Local Energy Decomposition of Open-Shell Molecular Systems in the Domain-Based Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2019, 15, 1616-1632. | 2.3 | 86 |

| # | Article | IF | Citations |
|---|---|---|---|
| 348 | Mg<sup>2+</sup>storage and mobility in anatase TiO<sub>2</sub>: the role of frustrated coordination. Journal of Materials Chemistry A, 2019, 7, 3704-3713. | 5.2 | 10 |
| 349 | Mapping the polymorphic transformation gateway vibration in crystalline 1,2,4,5-tetrabromobenzene. Chemical Science, 2019, 10, 1332-1341. | 3.7 | 26 |
| 350 | When hydrogen bonding overcomes Coulomb repulsion: from kinetic to thermodynamic stability of cationic dimers. Physical Chemistry Chemical Physics, 2019, 21, 8215-8220. | 1.3 | 29 |
| 351 | Mixed Layered Growth of Fullerene C<sub>60</sub> Self-Assembly on an Oxygen-Passivated Fe(001)-p(1 Ã— 1)O Surface. Journal of Physical Chemistry C, 2019, 123, 15477-15482. | 1.5 | 4 |
| 352 | New scaling relations to compute atom-in-material polarizabilities and dispersion coefficients: part 1. Theory and accuracy. RSC Advances, 2019, 9, 19297-19324. | 1.7 | 16 |
| 353 | Face, Notch, or Edge? Intermolecular dissociation energies of 1-naphthol complexes with linear molecules. Journal of Chemical Physics, 2019, 150, 234303. | 1.2 | 10 |
| 354 | The Doubleâ€Faced Nature of Hydrogen Bonding in Hydroxyâ€Functionalized Ionic Liquids Shown by Neutron Diffraction and Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2019, 58, 12887-12892. | 7.2 | 40 |
| 355 | Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie - International Edition, 2019, 58, 11078-11087. | 7.2 | 72 |
| 356 | Benchmarking the Accuracy of Seniority-Zero Wave Function Methods for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2019, 15, 4021-4035. | 2.3 | 15 |
| 357 | Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. Journal of Chemical Theory and Computation, 2019, 15, 3610-3622. | 2.3 | 85 |
| 358 | Structure Optimisation of Large Transitionâ€Metal Complexes with Extended Tightâ€Binding Methods. Angewandte Chemie, 2019, 131, 11195-11204. | 1.6 | 21 |
| 359 | Die zweigesichtige Natur der WasserstoffbrÃ¼ckenbindung in hydroxylfunktionalisierten ionischen FlÃ¼ssigkeiten, offenbart durch Neutronendiffraktometrie und Molekulardynamikâ€Simulation. Angewandte Chemie, 2019, 131, 13019-13024. | 1.6 | 5 |
| 360 | Single crystal structure, hydrogen bonding interaction, charge transfer and thermal properties of a new guanidine derivative crystal: Phosphate bis-guanidinoacetate. Journal of Molecular Structure, 2019, 1195, 883-890. | 1.8 | 1 |
| 361 | Exploring the chemical nature of super-heavy main-group elements by means of efficient plane-wave density-functional theory. Physical Chemistry Chemical Physics, 2019, 21, 18048-18058. | 1.3 | 31 |
| 362 | Boric acid-based ternary deep eutectic solvent for extraction and oxidative desulfurization of diesel fuel. Green Chemistry, 2019, 21, 3074-3080. | 4.6 | 151 |
| 363 | Interaction in Li@Fullerenes and Li+@Fullerenes: First Principle Insights to Li-Based Endohedral Fullerenes. Nanomaterials, 2019, 9, 630. | 1.9 | 23 |
| 364 | A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie - International Edition, 2019, 58, 9758-9769. | 7.2 | 41 |
| 365 | Deciphering the Origin of Enantioselectivity on the Cis-Cyclopropanation of Styrene with Enantiopure Di-chloro,Di-gold(I)-SEGPHOS Carbenoids Generated from Propargylic Esters. Journal of Organic Chemistry, 2019, 84, 7664-7673. | 1.7 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 366 | Accurate and Efficient ab Initio Calculations for Supramolecular Complexes: Symmetry-Adapted Perturbation Theory with Many-Body Dispersion. Journal of Physical Chemistry Letters, 2019, 10, 2706-2714. | 2.1 | 51 |
| 367 | Structure and Dynamics of Water at the Waterâ€“Air Interface Using First-Principles Molecular Dynamics Simulations. II. NonLocal vs Empirical van der Waals Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3836-3843. | 2.3 | 12 |
| 368 | A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122. | 1.2 | 697 |
| 369 | Spectroscopic characterization of non-covalent CuPc-GO system. Experiment and theory. Materials Chemistry and Physics, 2019, 231, 301-310. | 2.0 | 4 |
| 370 | Comparative studies on the effect of CB[8] on the charge transfer interaction. Theoretical Chemistry Accounts, 2019, 138, 1. | 0.5 | 2 |
| 371 | van der Waals interactions in DFT using Wannier functions without empirical parameters. Journal of Chemical Physics, 2019, 150, 164109. | 1.2 | 14 |
| 372 | Clarifying the multiple roles of confinement in zeolites: From stabilization of transition states to modification of internal diffusion rates. Journal of Catalysis, 2019, 372, 382-387. | 3.1 | 13 |
| 373 | Assessment of Density Functional Theory in Predicting Interaction Energies between Water and Polycyclic Aromatic Hydrocarbons: from Water on Benzene to Water on Graphene. Journal of Chemical Theory and Computation, 2019, 15, 2359-2374. | 2.3 | 18 |
| 374 | Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO2 and AlPO4 frameworks. Journal of Chemical Physics, 2019, 150, 094102. | 1.2 | 24 |
| 375 | A Variational Approach to London Dispersion Interactions without Density Distortion. Journal of Physical Chemistry Letters, 2019, 10, 1537-1541. | 2.1 | 9 |
| 377 | Quantum chemical exploration of new Ï€-electron systems: Capsule-formed dimers of polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2019, 725, 59-65. | 1.2 | 5 |
| 378 | Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. Journal of Chemical Theory and Computation, 2019, 15, 3250-3259. | 2.3 | 43 |
| 379 | London dispersion effects in the coordination and activation of alkanes in Ïƒ-complexes: a local energy decomposition study. Physical Chemistry Chemical Physics, 2019, 21, 11569-11577. | 1.3 | 54 |
| 380 | The role of dispersion and anharmonic corrections in conformational analysis of flexible molecules: the allyl group rotamerization of matrix isolated safrole. Physical Chemistry Chemical Physics, 2019, 21, 8352-8364. | 1.3 | 5 |
| 381 | The structure and racemization of 1,2-bis(pentaphenylphenyl)benzene. Tetrahedron, 2019, 75, 2778-2784. | 1.0 | 9 |
| 382 | Structure and adhesion energy of the (10.4) calcite/(001) ice Ih and (210) baryte/(001) ice Ih interfaces. CrystEngComm, 2019, 21, 2920-2928. | 1.3 | 3 |
| 383 | Equation of State of Fluid Methane from First Principles with Machine Learning Potentials. Journal of Chemical Theory and Computation, 2019, 15, 2574-2586. | 2.3 | 40 |
| 384 | Phase stability of intercalated V<sub>2</sub>O<sub>5</sub> battery cathodes elucidated through the Goldschmidt tolerance factor. Physical Chemistry Chemical Physics, 2019, 21, 7732-7744. | 1.3 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 385 | Advances in Density-Functional Calculations for Materials Modeling. Annual Review of Materials Research, 2019, 49, 1-30. | 4.3 | 87 |
| 386 | Anomalous Temperature Dependence of the Lowest-Frequency Lattice Vibration in Crystalline Î³-Aminobutyric Acid. Journal of Physical Chemistry A, 2019, 123, 2058-2064. | 1.1 | 24 |
| 387 | Sn-based deep eutectic solvents assisted synthesis of Sn and SnO2 supported hexagonal boron nitrides for adsorptive desulfurization. Chemical Engineering Research and Design, 2019, 144, 11-18. | 2.7 | 21 |
| 388 | GFN2-xTBâ€"An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. Journal of Chemical Theory and Computation, 2019, 15, 1652-1671. | 2.3 | 1,704 |
| 389 | A Simple Model for Halogen Bond Interaction Energies. Inorganics, 2019, 7, 19. | 1.2 | 11 |
| 390 | Effect of the exchangeâ€"correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€"Alder reactions: a reaction force constant analysis. Physical Chemistry Chemical Physics, 2019, 21, 7412-7428. | 1.3 | 31 |
| 391 | A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. Australian Journal of Chemistry, 2019, 72, 563. | 0.5 | 115 |
| 392 | Weak interaction between water molecule and different rank coals: a DFT-D3 study. International Journal of Oil, Gas and Coal Technology, 2019, 21, 91. | 0.1 | 2 |
| 393 | Extending and assessing composite electronic structure methods to the solid state. Journal of Chemical Physics, 2019, 151, 121101. | 1.2 | 21 |
| 394 | Emerging DFT Methods and Their Importance for Challenging Molecular Systems with Orbital Degeneracy. Computation, 2019, 7, 62. | 1.0 | 5 |
| 395 | Intermolecular interaction energies from fourth order many-body perturbation theory. Impact of individual electron correlation contributions. Journal of Chemical Physics, 2019, 151, 114105. | 1.2 | 1 |
| 396 | The axial/equatorial conformational landscape and intramolecular dispersion: new insights from the rotational spectra of monoterpenoids. Physical Chemistry Chemical Physics, 2019, 21, 26111-26116. | 1.3 | 14 |
| 397 | A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie, 2019, 131, 9860-9871. | 1.6 | 8 |
| 398 | Preparation and structure of 4-(dimethylamino)thiopivalophenone â€" intermolecular interactions in the crystal. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2019, 74, 825-831. | 0.3 | 1 |
| 399 | Modeling chemical reactions on surfaces: The roles of chemical bonding and van der Waals interactions. Progress in Surface Science, 2019, 94, 100561. | 3.8 | 39 |
| 400 | Ab Initio Calculations for Moleculeâ€"Surface Interactions with Chemical Accuracy. Accounts of Chemical Research, 2019, 52, 3502-3510. | 7.6 | 70 |
| 401 | Second-Order Exchange-Dispersion Energy Based on a Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 6712-6723. | 2.3 | 11 |
| 402 | sp-hybridized carbon allotrope molecular structures: An ongoing challenge for density-functional approximations. Journal of Chemical Physics, 2019, 151, 211104. | 1.2 | 29 |

| # | Article | IF | Citations |
|---|---|---|---|
| 407 | Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275. | 1.3 | 13 |
| 408 | Impact of dihydrogen bonding on lattice energies and sublimation enthalpies of crystalline [H<sub>2</sub>GaNH<sub>2</sub>]<sub>3</sub>, [H<sub>2</sub>BNH<sub>2</sub>]<sub>3</sub> and [H<sub>2</sub>GeCH<sub>2</sub>]<sub>3</sub>. RSC Advances, 2019, 9, 29448-29455. | 1.7 | 0 |
| 409 | A collection of forcefield precursors for metalâ€“organic frameworks. RSC Advances, 2019, 9, 36492-36507. | 1.7 | 21 |
| 410 | Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266. | 7.6 | 117 |
| 411 | Siliconâ€“Halogen Bond Activation in Mixed Si/Al Compounds and an Approach to Intramolecular Stabilized Silylium Ions. European Journal of Inorganic Chemistry, 2019, 2019, 693-711. | 1.0 | 6 |
| 412 | Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Assessment of Strengths and Weaknesses of End-Point Free Energy Methods. Journal of Chemical Information and Modeling, 2019, 59, 421-440. | 2.5 | 17 |
| 413 | Anionâ‹¯Ï€ interaction in oxoanion-graphene complex using coronene as model system: A DFT study. Computational and Theoretical Chemistry, 2019, 1147, 62-71. | 1.1 | 15 |
| 414 | Insights into the non-covalent interaction between modified nucleobases and graphene nanoflake from first-principles. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 107, 73-79. | 1.3 | 19 |
| 415 | Assessment of Newest Meta-GGA Hybrids for Late Transition Metal Reactivity: Fractional Charge and Fractional Spin Perspective. Journal of Physical Chemistry C, 2019, 123, 8047-8056. | 1.5 | 17 |
| 416 | Deriving bonding concepts for molecules, surfaces, and solids with energy decomposition analysis for extended systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1401. | 6.2 | 28 |
| 417 | The Niecke Biradicals and Their Congeners â€“ The Journey from Stable Biradicaloids to Their Utilization for the Design of Nonlinear Optical Properties. European Journal of Inorganic Chemistry, 2019, 2019, 1495-1506. | 1.0 | 22 |
| 418 | Understanding non-covalent interactions in larger molecular complexes from first principles. Journal of Chemical Physics, 2019, 150, 010901. | 1.2 | 56 |
| 419 | New Light on an Old Story: The Crystal Structure of Boron Tetrathiophosphate Revisited. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2019, 645, 267-271. | 0.6 | 11 |
| 420 | Partial and Complete Substitution of the 1,4-Benzenedicarboxylate Linker in UiO-66 with 1,4-Naphthalenedicarboxylate: Synthesis, Characterization, and H<sub>2</sub>-Adsorption Properties. Inorganic Chemistry, 2019, 58, 1607-1620. | 1.9 | 42 |
| 421 | O<sub>2</sub> Activation and Oxidative Dehydrogenation of Propane on Hexagonal Boron Nitride: Mechanism Revisited. Journal of Physical Chemistry C, 2019, 123, 2256-2266. | 1.5 | 42 |
| 422 | Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. Journal of Physical Chemistry Letters, 2019, 10, 358-368. | 2.1 | 90 |
| 423 | Performance of van der Waals DFT approaches for helium diffraction on metal surfaces. Journal of Physics Condensed Matter, 2019, 31, 135901. | 0.7 | 4 |
| 424 | Quantum chemical exploration of dimeric forms of polycyclic aromatic hydrocarbons, naphthalene, perylene, and coronene. Chemical Physics Letters, 2019, 716, 147-154. | 1.2 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 425 | Second-Order Dispersion Energy Based on Multireference Description of Monomers. Journal of Chemical Theory and Computation, 2019, 15, 1016-1027. | 2.3 | 17 |
| 426 | Developments in the Atomistic Modelling of Catalytic Processes for the Production of Platform Chemicals from Biomass. ChemCatChem, 2019, 11, 357-367. | 1.8 | 3 |
| 427 | The electronic structure and physicochemical property of boron nitridene. Journal of Molecular Graphics and Modelling, 2020, 94, 107475. | 1.3 | 2 |
| 428 | The [4+2]â€Cycloaddition of Î±â€Nitrosoalkenes with Thiochalcones as a Prototype of Periselective Heteroâ€Dielsâ€“Alder Reactionsâ€”Experimental and Computational Studies. Chemistry - A European Journal, 2020, 26, 237-248. | 1.7 | 16 |
| 429 | Finding chemical concepts in the Hilbert space: Coupled cluster analyses of noncovalent interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1442. | 6.2 | 56 |
| 430 | Alkali and Alkalineâ€Earth Cations in Complexes with Small Bioorganic Ligands: Abâ€…Initio Benchmark Calculations and Bond Energy Decomposition. ChemPhysChem, 2020, 21, 99-112. | 1.0 | 10 |
| 431 | Ab Initio Investigation of CO2 Adsorption on 13-Atom 4d Clusters. Journal of Chemical Information and Modeling, 2020, 60, 537-545. | 2.5 | 20 |
| 432 | Vibrational Response of Felodipine in the THz Domain: Optical and Neutron Spectroscopy Versus Plane-Wave DFT Modeling. Journal of Infrared, Millimeter, and Terahertz Waves, 2020, 41, 1301-1336. | 1.2 | 7 |
| 433 | Dissecting intermolecular interactions in the condensed phase of ibuprofen and related compounds: the specific role and quantification of hydrogen bonding and dispersion forces. Physical Chemistry Chemical Physics, 2020, 22, 4896-4904. | 1.3 | 13 |
| 434 | Random Phase Approximation Applied to Many-Body Noncovalent Systems. Journal of Chemical Theory and Computation, 2020, 16, 427-442. | 2.3 | 12 |
| 435 | A theoretical indicator of transition-metal nanoclusters applied in the carbon nanotube nucleation process: a DFT study. Dalton Transactions, 2020, 49, 492-503. | 1.6 | 10 |
| 436 | Prediction of correct intermolecular interactions in host-guest systems involving cyclodextrins. Journal of Molecular Structure, 2020, 1205, 127517. | 1.8 | 6 |
| 437 | Empirical Doubleâ€Hybrid Density Functional Theory: A â€˜Third Wayâ€™ in Between WFT and DFT. Israel Journal of Chemistry, 2020, 60, 787-804. | 1.0 | 129 |
| 438 | Quantum Chemical Exploration of Intermolecular Reactions of Acetylene. Journal of Computational Chemistry, 2020, 41, 687-697. | 1.5 | 2 |
| 439 | Recent developments in symmetryâ€adapted perturbation theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1452. | 6.2 | 102 |
| 440 | Cause, Regulation and Utilization of Dye Aggregation in Dye-Sensitized Solar Cells. Molecules, 2020, 25, 4478. | 1.7 | 30 |
| 441 | Conformational preferences of cationic Î²-peptide in water studied by CCSD(T), MP2, and DFT methods. Heliyon, 2020, 6, e04721. | 1.4 | 4 |
| 442 | On the hydrogen storage performance of Cu-doped and Cu-decorated graphene quantum dots: a computational study. Theoretical Chemistry Accounts, 2020, 139, 1. | 0.5 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 443 | Structural Stability of the CO<sub>2</sub>@sI Hydrate: a Bottomâ€Up Quantum Chemistry Approach on the Guestâ€Cage and Interâ€Cage Interactions. ChemPhysChem, 2020, 21, 2618-2628. | 1.0 | 9 |
| 444 | From Sâ€“Oâ€“S to Bâ€“Oâ€“S to Bâ€“Oâ€“B Bridges: Ba[B(S<sub>2</sub>O<sub>7</sub>)<sub>2</sub>]<sub>2</sub> as a Model System for the Structural Diversity in Borosulfate Chemistry. Inorganic Chemistry, 2020, 59, 15180-15188. | 1.9 | 14 |
| 445 | Reactions of Alâ€N Based Active Lewis Pairs with Ketones and 1,2â€Diketones: Insertion into Alâ€N Bonds, Câ€C and Câ€N Bond Formation and a Tricyclic Saturated Tetraaza Compound. European Journal of Inorganic Chemistry, 2020, 2020, 3760-3770. | 1.0 | 7 |
| 446 | Cost-effective composite methods for large-scale solid-state calculations. Faraday Discussions, 2020, 224, 292-308. | 1.6 | 13 |
| 447 | Probing Mg Intercalation in the Tetragonal Tungsten Bronze Framework V<sub>4</sub>Nb<sub>18</sub>O<sub>55</sub>. Inorganic Chemistry, 2020, 59, 9783-9797. | 1.9 | 7 |
| 448 | Protobranching as repulsion-induced attraction: a prototype for geminal stabilization. Physical Chemistry Chemical Physics, 2020, 22, 16998-17006. | 1.3 | 1 |
| 449 | Density Functional Theories and Coordination Chemistry. , 2020, , . | | 2 |
| 450 | Cohesiveness and Nondiffusive Rotational Jump Dynamics of Protic Ionic Liquid from Dispersion-Corrected FPMD Simulations. Journal of Physical Chemistry B, 2020, 124, 10752-10765. | 1.2 | 5 |
| 451 | Synthesis of Platinum-Containing Conjugated Polymers Bearing Optically Active Amide Groups: A Mechanistic Study of Chiral Aggregation. Macromolecules, 2020, 53, 11077-11088. | 2.2 | 12 |
| 452 | Liquid water contains the building blocks of diverse ice phases. Nature Communications, 2020, 11, 5757. | 5.8 | 50 |
| 453 | Efficient Calculation of Small Molecule Binding in Metalâ€Organic Frameworks and Porous Organic Cages. Journal of Physical Chemistry C, 2020, 124, 27529-27541. | 1.5 | 32 |
| 454 | Symmetry/Asymmetry of the NHN Hydrogen Bond in Protonated 1,8-Bis(dimethylamino)naphthalene. Symmetry, 2020, 12, 1924. | 1.1 | 8 |
| 455 | The usefulness of energy decomposition schemes to rationalize hostâ€guest interactions. Dalton Transactions, 2020, 49, 17457-17471. | 1.6 | 13 |
| 456 | Diffusion, permeation and solubility of hydrogen, deuterium and tritium in crystalline tungsten: First principles DFT simulations. International Journal of Hydrogen Energy, 2020, 45, 29095-29109. | 3.8 | 27 |
| 457 | A Second Modification of Beryllium Bromide: Î²-BeBr2. Inorganic Chemistry, 2020, 59, 16783-16788. | 1.9 | 8 |
| 458 | What Does the BrÃ¸nsted Slope Measure in the Phosphoryl Transfer Transition State?. ACS Catalysis, 2020, 10, 13932-13945. | 5.5 | 3 |
| 459 | Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries. Journal of Chemical Physics, 2020, 153, 054121. | 1.2 | 11 |
| 460 | Synthesis of Alkyl Silanes via Reaction of Unactivated Alkyl Chlorides and Triflates with Silyl Lithium Reagents. Organic Letters, 2020, 22, 6568-6572. | 2.4 | 17 |

| # | Article | IF | Citations |
|---|---|---|---|
| 461 | The interaction nature between hollow silica-based porous ionic liquids and CO2: A DFT study. Journal of Molecular Graphics and Modelling, 2020, 100, 107694. | 1.3 | 21 |
| 462 | Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507. | 1.3 | 25 |
| 463 | Bingelâ€“Hirsch Addition of Diethyl Bromomalonate to Ionâ€Encapsulated Fullerenes M@C 60 (M=Ã˜, Li + ,) Tj ETQq0 0 0 rgBT /Overloc | 1.7 | 6 |
| 464 | Next-Generation Nonlocal van der Waals Density Functional. Journal of Chemical Theory and Computation, 2020, 16, 5893-5911. | 2.3 | 57 |
| 465 | Synthesisâ€Controlled Polymorphism and Optical Properties of Phyllosilicateâ€Analogous Borosulfates M [B 2 (SO 4 ) 4 ] ( M =Mg, Co). Chemistry - A European Journal, 2020, 26, 14745-14753. | 1.7 | 20 |
| 466 | Basis Set Extrapolations for Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 5712-5722. | 2.3 | 13 |
| 467 | Design of novel conjugated microporous polymers for efficient adsorptive desulfurization of small aromatic sulfur molecules. Journal of Molecular Graphics and Modelling, 2020, 101, 107734. | 1.3 | 3 |
| 468 | Two effective computational schemes for a prototype of an excitable system. AIP Advances, 2020, 10, 105120. | 0.6 | 22 |
| 469 | PubChemQC PM6: Data Sets of 221 Million Molecules with Optimized Molecular Geometries and Electronic Properties. Journal of Chemical Information and Modeling, 2020, 60, 5891-5899. | 2.5 | 36 |
| 470 | Role of Methane as a Second Guest Component in Thermodynamic Stability and Isomer Selectivity of Butane Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 18474-18481. | 1.5 | 17 |
| 471 | Theoretical prediction of F-doped hexagonal boron nitride: A promising strategy to enhance the capacity of adsorptive desulfurization. Journal of Molecular Graphics and Modelling, 2020, 101, 107715. | 1.3 | 11 |
| 472 | DFT<scp>â€D4</scp> counterparts of leading <scp>metaâ€</scp>generalizedâ€gradient approximation and hybrid density functionals for energetics and geometries. Journal of Computational Chemistry, 2020, 41, 2562-2572. | 1.5 | 61 |
| 473 | Free-energy landscape of polymer-crystal polymorphism. Soft Matter, 2020, 16, 9683-9692. | 1.2 | 9 |
| 474 | How Much Dispersion Energy Is Included in the Multiconfigurational Interaction Energy?. Journal of Chemical Theory and Computation, 2020, 16, 6280-6293. | 2.3 | 8 |
| 475 | Cyclic Octamer of Hydroxylâ€functionalized Cations with Net Charge Q =+8 e Kinetically Stabilized by a â€˜Molecular Islandâ€™ of Cooperative Hydrogen Bonds. ChemPhysChem, 2020, 21, 2411-2416. | 1.0 | 3 |
| 476 | Accuracy of intermolecular interaction energies, particularly those of hetero-atom containing molecules obtained by DFT calculations with Grimme's D2, D3 and D3BJ dispersion corrections. Physical Chemistry Chemical Physics, 2020, 22, 22508-22519. | 1.3 | 68 |
| 477 | Bond Dissociation Energies in the Gas Phase for Large Molecular Ions by Threshold Collision-Induced Dissociation Experiments: Stretching the Limits. Journal of Physical Chemistry A, 2020, 124, 8692-8707. | 1.1 | 11 |
| 478 | Multifidelity Statistical Machine Learning for Molecular Crystal Structure Prediction. Journal of Physical Chemistry A, 2020, 124, 8065-8078. | 1.1 | 38 |

| # | Article | IF | Citations |
|---|---|---|---|
| 479 | Modeling Biologically Important NHÂ·Â·Â·Ï€ Interactions Using peri-Disubstituted Naphthalenes. Journal of Organic Chemistry, 2020, 85, 12468-12481. | 1.7 | 8 |
| 480 | Crystalline Molecular Standards for Low-Frequency Vibrational Spectroscopies. Journal of Infrared, Millimeter, and Terahertz Waves, 2020, 41, 1284-1300. | 1.2 | 9 |
| 481 | N<sup>5</sup>-Scaling Excited-State-Specific Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 6132-6141. | 2.3 | 14 |
| 482 | Differences in the Nature of the Phosphoryl Transfer Transition State in Protein Phosphatase 1 and Alkaline Phosphatase: Insights from QM Cluster Models. Journal of Physical Chemistry B, 2020, 124, 9371-9384. | 1.2 | 4 |
| 483 | Influence of Local Inhomogeneities and the Electrochemical Environment on the Oxygen Reduction Reaction on Pt-Based Electrodes: A DFT Study. Journal of Physical Chemistry C, 2020, 124, 27604-27613. | 1.5 | 10 |
| 484 | Reactivity and Selectivity Controlling Factors in the Pd/Dialkylbiarylphosphine-Catalyzed Câ€“C Cleavage/Cross-Coupling of an N-Fused Bicyclo Î±-Hydroxy-Î²-Lactam. Journal of the American Chemical Society, 2020, 142, 21140-21152. | 6.6 | 20 |
| 485 | Local bottom-up effective theory of nonlocal electronic interactions. Physical Review B, 2020, 102, . | 1.1 | 2 |
| 486 | Many-Body Dispersion. Chemical Reviews, 2020, 120, 12343-12356. | 23.0 | 16 |
| 487 | Clusters of Hydroxyl-Functionalized Cations Stabilized by Cooperative Hydrogen Bonds: The Role of Polarizability and Alkyl Chain Length. Molecules, 2020, 25, 4972. | 1.7 | 12 |
| 488 | Ab Initio Study of Chiral Discrimination in the Glycidol Dimer. Journal of Physical Chemistry A, 2020, 124, 9436-9450. | 1.1 | 3 |
| 489 | Genetic Parameterization of Interfacial Force Fields Based on Classical Bulk Force Fields and Ab Initio Data: Application to the Methanol-ZnO Interfaces. Journal of Chemical Information and Modeling, 2020, 60, 6033-6043. | 2.5 | 4 |
| 490 | Theoretical free energy profile and benchmarking of functionals for amino-thiourea organocatalyzed nitro-Michael addition reaction. Physical Chemistry Chemical Physics, 2020, 22, 11529-11536. | 1.3 | 20 |
| 491 | Inclusion of Van der Waals Interactions in DFT using Wannier Functions without empirical parameters. EPJ Web of Conferences, 2020, 230, 00010. | 0.1 | 1 |
| 492 | Vibrational mode frequency correction of liquid water in density functional theory molecular dynamics simulations with van der Waals correction. Physical Chemistry Chemical Physics, 2020, 22, 12785-12793. | 1.3 | 9 |
| 493 | The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111. | 1.2 | 133 |
| 494 | The ORCA quantum chemistry program package. Journal of Chemical Physics, 2020, 152, 224108. | 1.2 | 1,915 |
| 495 | Rationalization of Lattice Thermal Expansion for Beta-Blocker Organic Crystals. Crystals, 2020, 10, 350. | 1.0 | 6 |
| 496 | SQM/COSMO Scoring Function: Reliable Quantumâ€Mechanical Tool for Sampling and Ranking in Structureâ€Based Drug Design. ChemPlusChem, 2020, 85, 2362-2371. | 1.3 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 497 | Discovery and design of soft polymeric bio-inspired materials with multiscale simulations and artificial intelligence. Journal of Materials Chemistry B, 2020, 8, 6562-6587. | 2.9 | 44 |
| 498 | London dispersion forces without density distortion: a path to first principles inclusion in density functional theory. Faraday Discussions, 2020, 224, 145-165. | 1.6 | 4 |
| 499 | Electronic structures and bonding of graphdiyne and its BN analogs: Transition from quasi-planar to planar sheets. Journal of Alloys and Compounds, 2020, 846, 155987. | 2.8 | 5 |
| 500 | Intermolecular dissociation energies of 1-naphthol complexes with large dispersion-energy donors: Decalins and adamantane. Journal of Chemical Physics, 2020, 152, 104304. | 1.2 | 3 |
| 501 | Semiclassical Dispersion Corrections Efficiently Improve Multiconfigurational Theory with Short-Range Density-Functional Dynamic Correlation. Journal of Physical Chemistry A, 2020, 124, 2834-2841. | 1.1 | 4 |
| 502 | Carbon dioxide gas sensing, capture, and storage potential of calcium oxide surface and single walled carbon nanotube: insights from ab initio simulation. Journal of Physics Condensed Matter, 2020, 32, 245901. | 0.7 | 3 |
| 503 | Conformational Landscapes and Infrared Spectra of Gas-phase Interstellar Molecular Clusters [(C3H3N)(CH3OH)n, n = 1â€“4]. Journal of Physical Chemistry A, 2020, 124, 2398-2407. | 1.1 | 6 |
| 504 | Long-range-corrected multiconfiguration density functional with the on-top pair density. Journal of Chemical Physics, 2020, 152, 094102. | 1.2 | 15 |
| 505 | Modelling the bulk properties of ambient pressure polymorphs of zirconia. Physical Chemistry Chemical Physics, 2020, 22, 6660-6676. | 1.3 | 16 |
| 506 | Electronic and Vibrational Contributions to the Bulk Stabilities of Trivalent 3d Transition Metal Oxyhydroxides from Electronic Structure Calculations. Journal of Physical Chemistry C, 2020, 124, 7500-7510. | 1.5 | 0 |
| 507 | Extension and evaluation of the D4 London-dispersion model for periodic systems. Physical Chemistry Chemical Physics, 2020, 22, 8499-8512. | 1.3 | 138 |
| 508 | Tridentate Ligand with Three Carbanions as Donor Atoms: Formation of Dinuclear, Heptacyclic Complexes of Boron, Aluminum, or Gallium with Bâ€“Câ€“B, Alâ€“Câ€“Al, or Gaâ€“Câ€“Ga Three-Centerâ€“Two-Electron Bonds. Inorganic Chemistry, 2020, 59, 5558-5563. | 1.9 | 0 |
| 509 | Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. Journal of Physical Chemistry Letters, 2020, 11, 2298-2302. | 2.1 | 17 |
| 510 | Origins of fast diffusion of water dimers on surfaces. Nature Communications, 2020, 11, 1689. | 5.8 | 39 |
| 511 | Roadmap on post-DFT methods for nanoscience. Nano Futures, 2020, 4, 032004. | 1.0 | 4 |
| 512 | Making Base-Assisted Câ€“H Bond Activation by Cp*Co(III) Effective: A Noncovalent Interaction-Inclusive Theoretical Insight and Experimental Validation. Organometallics, 2020, 39, 2609-2629. | 1.1 | 13 |
| 513 | Interactions of CO<sub>2</sub> with cluster models of <scp>metalâ€“organic</scp> frameworks. Journal of Computational Chemistry, 2020, 41, 2066-2083. | 1.5 | 0 |
| 514 | New Reactivity Patterns in 3Hâ€Phosphaallene Chemistry [Arylâ€P=C=C(H)â€tBu]: Hydroboration of the C=C Bond, Deprotonation and Trimerisation. Chemistry - A European Journal, 2020, 26, 15977-15988. | 1.7 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 515 | Inaccurate Conformational Energies Still Hinder Crystal Structure Prediction in Flexible Organic Molecules. Crystal Growth and Design, 2020, 20, 4875-4881. | 1.4 | 48 |
| 516 | A computational chemistry approach to modelling conducting polymers in ionic liquids for next generation batteries. Energy Reports, 2020, 6, 198-208. | 2.5 | 13 |
| 517 | Soot inception: A DFT study of ÏƒÂ and ÏÂ€ dimerization of resonantly stabilized aromatic radicals. Fuel, 2020, 279, 118491. | 3.4 | 19 |
| 518 | Aspects of Phosphaallene Chemistry: Heat-Induced Formation of 1,2-Dihydrophosphetes by Intramolecular Nucleophilic Aromatic Substitution and Photochemical Generation of Tricyclic Phosphiranes. Journal of Organic Chemistry, 2020, 85, 14315-14332. | 1.7 | 10 |
| 519 | Performance study of the electronic and optical parameters of thermally activated delayed fluorescence nanosized emitters (CCX-I and CCX-II) via DFT, SCC-DFTB and B97-3c approaches. Journal of Nanostructure in Chemistry, 2020, 10, 115-124. | 5.3 | 11 |
| 520 | AlkoxyalleneâÂ€Based LANCA ThreeâÂ€Component Synthesis of 1,2â€Diketones, Quinoxalines, and Unique Isoindenone Dimers and a Computational Study of the Isoindenone Dimerization. European Journal of Organic Chemistry, 2020, 2020, 1753-1763. | 1.2 | 4 |
| 521 | Structural, electronic, and vibrational properties of choline halides. Materials Chemistry and Physics, 2020, 246, 122787. | 2.0 | 4 |
| 522 | Benchmarking of Semiempirical Quantum-Mechanical Methods on Systems Relevant to Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1453-1460. | 2.5 | 45 |
| 523 | Thermal spin crossover in Fe(<scp>ii</scp>) and Fe(<scp>iii</scp>). Accurate spin state energetics at the solid state. Physical Chemistry Chemical Physics, 2020, 22, 4938-4945. | 1.3 | 32 |
| 524 | Molecular Design of Aromatic Polythionoesters. ACS Omega, 2020, 5, 3016-3029. | 1.6 | 3 |
| 525 | Abundant new solutions of the transmission of nerve impulses of an excitable system. European Physical Journal Plus, 2020, 135, 1. | 1.2 | 25 |
| 526 | Benchmark Experimental Gas-Phase Intermolecular Dissociation Energies by the SEP-R2PI Method. Annual Review of Physical Chemistry, 2020, 71, 189-211. | 4.8 | 8 |
| 527 | Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory Based Ab Initio Molecular Dynamics. 1. Theory, Algorithm, and Performance. Journal of Chemical Theory and Computation, 2020, 16, 3757-3785. | 2.3 | 29 |
| 528 | B(C 6 F 5 ) 3 /Chiral Phosphoric Acid Catalyzed Ketimineâ€“Ene Reaction of 2â€Arylâ€3 H â€indolâ€3â€ones and Î±â€Methylstyrenes. Angewandte Chemie, 2020, 132, 4580-4586. | 1.6 | 10 |
| 529 | Controlling â€œlikeâ€“likesâ€“likeâ€•charge attraction in hydroxy-functionalized ionic liquids by polarizability of the cations, interaction strength of the anions and varying alkyl chain length. Physical Chemistry Chemical Physics, 2020, 22, 2763-2774. | 1.3 | 29 |
| 530 | Water structures on a Pt(111) electrode from ab initio molecular dynamic simulations for a variety of electrochemical conditions. Physical Chemistry Chemical Physics, 2020, 22, 10431-10437. | 1.3 | 65 |
| 531 | Insight into the Expanded Mislinked Porphyrins with High Second Order Nonlinear Optical Response. Journal of Physical Chemistry A, 2020, 124, 955-965. | 1.1 | 18 |
| 532 | Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq1 1 0.784314 rgBT /O | 1.1 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 533 | B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>/Chiral Phosphoric Acid Catalyzed Ketimineâ€“Ene Reaction of 2â€Arylâ€3Hâ€indolâ€3â€ones and Îąâ€Methylstyrenes. Angewandte Chemie - International Edition, 2020, 59, 4550-4556. | 12.2 | 40 |
| 534 | Evolutionary Algorithmâ€based Crystal Structure Prediction for Gold(I) Fluoride. ChemPhysChem, 2020, 21, 802-808. | 1.0 | 8 |
| 535 | A Short Review of Current Computational Concepts for High-Pressure Phase Transition Studies in Molecular Crystals. Crystals, 2020, 10, 81. | 1.0 | 19 |
| 536 | Feâ€porphyrin on Co(001) and Cu(001): A Comparative Dispersionâ€augmented Density Functional Theory Study. Israel Journal of Chemistry, 2020, 60, 870-875. | 1.0 | 0 |
| 537 | Quantum chemical exploration of polymerized forms of polycyclic aromatic hydrocarbons: D6h tetramer and polymer of coronene. Chemical Physics Letters, 2020, 747, 137366. | 1.2 | 3 |
| 538 | Introduction: Bond Specific Spectroscopy of Peptides and Proteins. Chemical Reviews, 2020, 120, 3231-3232. | 23.0 | 1 |
| 539 | Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metalâ€organic frameworks and in acidic zeolites. Physical Chemistry Chemical Physics, 2020, 22, 7577-7585. | 1.3 | 30 |
| 540 | What is â€œmany-bodyâ€•dispersion and should I worry about it?. Physical Chemistry Chemical Physics, 2020, 22, 8266-8276. | 1.3 | 30 |
| 541 | Computational simulations of the couple Boitiâ€“Leonâ€“Pempinelli (BLP) system and the (3+1)-dimensional Kadomtsevâ€“Petviashvili (KP) equation. AIP Advances, 2020, 10, . | 0.6 | 28 |
| 542 | The many-body expansion approach to ab initio calculation of electric field gradients in molecular crystals. Journal of Chemical Physics, 2020, 152, 124105. | 1.2 | 5 |
| 543 | Density Functional Model for van der Waals Interactions: Unifying Many-Body Atomic Approaches with Nonlocal Functionals. Physical Review Letters, 2020, 124, 146401. | 2.9 | 53 |
| 544 | Evaluation of bismuth-based dispersion energy donors â€“ synthesis, structure and theoretical study of 2-biphenylbismuth(<scp>iii</scp>) derivatives. Physical Chemistry Chemical Physics, 2020, 22, 10189-10211. | 1.3 | 5 |
| 545 | Theoretical investigation of para aminoâ€dichloro chalcone isomers, part I: A DFT structureâ€”stability study. Journal of Physical Organic Chemistry, 2020, 33, e4073. | 0.9 | 3 |
| 546 | Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3530-3542. | 2.3 | 2 |
| 547 | The H2S dimer revisited â€“ Insights from wave-function and density functional theory methods. Ab initio molecular dynamics simulations of liquid H2S. Computational and Theoretical Chemistry, 2020, 1180, 112821. | 1.1 | 3 |
| 548 | Benchmarking Cationâ€Îľ Interactions: Assessment of Density Functional Theory and MÃžllerâ€“Plesset Second-Order Perturbation Theory Calculations with Optimized Basis Sets (<scp>mp</scp>2<sup>mod</sup>) for Complexes of Benzene, Phenol, and Catechol with Na<sup>+</sup>, K<sup>+</sup>, Rb<sup>+</sup>, and Cs<sup>+</sup>. Journal of Physical Chemistry A, 2020, 124, 3445-3459. | 1.1 | 20 |
| 549 | CO, NO, and SO adsorption on Ni nanoclusters: a DFT investigation. Dalton Transactions, 2020, 49, 6407-6417. | 1.6 | 27 |
| 550 | The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107. | 1.2 | 603 |

| # | Article | IF | Citations |
|---|---|---|---|
| 551 | London Dispersion in Alkanen als LÃ¶sungsmittel. Angewandte Chemie, 2021, 133, 792-799. | 1.6 | 3 |
| 552 | Substituent effect on ESIPT and hydrogen bond mechanism of N-(8-Quinolyl) salicylaldimine: A detailed theoretical exploration. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 245, 118937. | 2.0 | 11 |
| 553 | Intermolecular interaction characteristics of the all-carboatomic ring, cyclo[18]carbon: Focusing on molecular adsorption and stacking. Carbon, 2021, 171, 514-523. | 5.4 | 333 |
| 554 | London Dispersion in Alkane Solvents. Angewandte Chemie - International Edition, 2021, 60, 779-786. | 7.2 | 22 |
| 555 | Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639. | 1.7 | 25 |
| 556 | On the formation of sandwich complexes of aromatic inorganic linker: A DFT-D3 approach. Polyhedron, 2021, 194, 114911. | 1.0 | 2 |
| 557 | Guiding the design of practical MTW zeolite catalysts: An integrated experimental-theoretical perspective. Microporous and Mesoporous Materials, 2021, 312, 110810. | 2.2 | 10 |
| 558 | High performance global exploration of isomers and isomerization channels on quantum chemical potential energy surface of <scp>H<sub>5</sub>C<sub>2</sub>NO<sub>2</sub></scp>. Journal of Computational Chemistry, 2021, 42, 192-204. | 1.5 | 5 |
| 559 | London Dispersion Interactions Rather than Steric Hindrance Determine the Enantioselectivity of the Coreyâ€“Bakshiâ€“Shibata Reduction. Angewandte Chemie - International Edition, 2021, 60, 4823-4832. | 7.2 | 57 |
| 560 | Understanding endohedral behaviors of ten-electron atomic and cluster system inside C60 from first-principles. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 127, 114532. | 1.3 | 7 |
| 561 | Atomic scale mechanism of clay minerals dissolution revealed by ab initio simulations. Geochimica Et Cosmochimica Acta, 2021, 293, 438-460. | 1.6 | 13 |
| 562 | London Dispersion Interactions Rather than Steric Hindrance Determine the Enantioselectivity of the Coreyâ€“Bakshiâ€“Shibata Reduction. Angewandte Chemie, 2021, 133, 4873-4882. | 1.6 | 10 |
| 563 | Computational Methods in Heterogeneous Catalysis. Chemical Reviews, 2021, 121, 1007-1048. | 23.0 | 198 |
| 564 | Experimental and Computational Analysis of CO<sub>2</sub> Addition Reactions Relevant to Copper-Catalyzed Boracarboxylation of Vinyl Arenes: Evidence for a Phosphine-Promoted Mechanism. Organometallics, 2021, 40, 23-37. | 1.1 | 16 |
| 565 | Planar Tetracoordinate Silicon in Organic Molecules As Carbenoidâ€Type Amphoteric Centers: A Computational Study. Chemistry - A European Journal, 2021, 27, 1402-1409. | 1.7 | 10 |
| 566 | <scp>NCIPLOT</scp> and the analysis of noncovalent interactions using the reduced density gradient. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1497. | 6.2 | 56 |
| 567 | Computational evidence of glycosyl cations. Organic and Biomolecular Chemistry, 2021, 19, 2350-2365. | 1.5 | 14 |
| 568 | Cyclopeptides from the Mushroom Pathogen Fungus Cladobotryum varium. Journal of Natural Products, 2021, 84, 327-338. | 1.5 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 569 | Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648. | 1.3 | 31 |
| 570 | Tuning the first hyperpolarizability of hexaphyrins with different connections of mislinked pyrrole units: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 8489-8499. | 1.3 | 10 |
| 571 | Towards the understanding of halogenation in peptide hydrogels: a quantum chemical approach. Materials Advances, 2021, 2, 4792-4803. | 2.6 | 3 |
| 572 | Assessing the Applicability of the Geometric Counterpoise Correction in B2PLYP/Double-Î¶ Calculations for Thermochemistry, Kinetics, and Noncovalent Interactions*. Australian Journal of Chemistry, 2021, , . | 0.5 | 2 |
| 573 | Rubrene untwisted: common density functional theory calculations overestimate its deviant tendencies. Journal of Materials Chemistry C, 2021, 9, 2848-2857. | 2.7 | 20 |
| 574 | The hierarchy of ab initio and DFT methods for describing an intramolecular non-covalent Siâ‹¯N contact in the silicon compounds using electron diffraction geometries. Physical Chemistry Chemical Physics, 2021, 23, 2762-2774. | 1.3 | 4 |
| 575 | Spectroscopic evidence of the Câ€“N covalent bond formed between two interstellar molecules (ISM): acrylonitrile and ammonia. Physical Chemistry Chemical Physics, 2021, 23, 9672-9678. | 1.3 | 11 |
| 576 | Computational Coordination Chemistry. , 2021, , 241-255. | | 4 |
| 577 | Insights into the Mechanism of Low-Valent Cobalt-Catalyzed Câ€“H Activation. ACS Catalysis, 2021, 11, 1505-1515. | 5.5 | 32 |
| 578 | Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. Physical Chemistry Chemical Physics, 2021, 23, 8962-9048. | 1.3 | 47 |
| 579 | Exploring CO<sub>2</sub>@sI Clathrate Hydrates as CO<sub>2</sub> Storage Agents by Computational Density Functional Approaches. ChemPhysChem, 2021, 22, 359-369. | 1.0 | 11 |
| 580 | Quantum-mechanical exploration of the phase diagram of water. Nature Communications, 2021, 12, 588. | 5.8 | 32 |
| 581 | The power of trichlorosilylation: isolable trisilylated allyl anions, allyl radicals, and allenyl anions. Chemical Science, 2021, 12, 12419-12428. | 3.7 | 4 |
| 582 | Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in Pseudomonads Demonstrating Siderophore-like Activity. ACS Infectious Diseases, 2021, 7, 544-551. | 1.8 | 16 |
| 583 | Combination of â€œButtressingâ€•and â€œClothespinâ€•Effects for Reaching the Shortest NHN Hydrogen Bond in Proton Sponge Cations. Journal of Organic Chemistry, 2021, 86, 3637-3647. | 1.7 | 14 |
| 584 | Single-Point Hessian Calculations for Improved Vibrational Frequencies and Rigid-Rotor-Harmonic-Oscillator Thermodynamics. Journal of Chemical Theory and Computation, 2021, 17, 1701-1714. | 2.3 | 49 |
| 585 | Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states. Journal of Chemical Physics, 2021, 154, 064108. | 1.2 | 37 |
| 586 | r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103. | 1.2 | 290 |

| # | Article | IF | Citations |
|---|---|---|---|
| 587 | r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. Journal of Chemical Physics, 2021, 154, 061101. | 1.2 | 70 |
| 588 | Revealing the Dynamic Process of Ion Pair Recognition by Calix[4]pyrrole: A Case Study of Cesium Chloride. Journal of Physical Chemistry Letters, 2021, 12, 3253-3259. | 2.1 | 6 |
| 589 | Identifying Barrierless Mechanisms for Benzene Formation in the Interstellar Medium Using Permutationally Invariant Reaction Discovery. Journal of Chemical Theory and Computation, 2021, 17, 2307-2322. | 2.3 | 8 |
| 590 | Dispersion without Many-Body Density Distortion: Assessment on Atoms and Small Molecules. Journal of Chemical Theory and Computation, 2021, 17, 2283-2293. | 2.3 | 1 |
| 591 | Relaxor ferroelectricity in the polar M2P-TCNQ charge-transfer crystal at the neutral-ionic interface. Physical Review B, 2021, 103, . | 1.1 | 3 |
| 592 | Ni/Cu-catalyzed silylation of allylic alcohol: Theoretical studies on the mechanisms, regioselectivity, and role of ligand. Molecular Catalysis, 2021, 504, 111456. | 1.0 | 1 |
| 593 | Interplay between London Dispersion, Hubbard U, and Metastable States for Uranium Compounds. Journal of Physical Chemistry A, 2021, 125, 2791-2799. | 1.1 | 4 |
| 594 | Dataset of noncovalent intermolecular interaction energy curves for 24 small high-spin open-shell dimers. Journal of Chemical Physics, 2021, 154, 134106. | 1.2 | 5 |
| 595 | Hetero-Diels-Alder Reactions of In Situ-Generated Azoalkenes with Thioketones; Experimental and Theoretical Studies. Molecules, 2021, 26, 2544. | 1.7 | 9 |
| 596 | A New Ligand Design Based on London Dispersion Empowers Chiral Bismuthâ€“Rhodium Paddlewheel Catalysts. Journal of the American Chemical Society, 2021, 143, 5666-5673. | 6.6 | 42 |
| 597 | Adsorption of polycyclic aromatic hydrocarbons on FeOOH polymorphs: A theoretical study. Surface Science, 2021, 706, 121795. | 0.8 | 7 |
| 598 | Effects of edge substitution of subazaphenalenephthalocyanine with electron withdrawing and/or donating groups on electronic and optical properties: A DFT/TDDFT study. Materials Chemistry and Physics, 2021, 263, 124420. | 2.0 | 4 |
| 599 | Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€: Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie, 2021, 133, 13252-13257. | 1.6 | 4 |
| 600 | Effect of anion identity on ion association and dynamics of sodium ions in non-aqueous glyme based electrolytesâ€”OTf vs TFSI. Journal of Chemical Physics, 2021, 154, 184505. | 1.2 | 8 |
| 601 | The role of long-range interactions on the selectivity of gaseous molecule-surface scattering. Chemical Physics Letters, 2021, 770, 138444. | 1.2 | 4 |
| 602 | Noncovalent Interactions from Models for the MÃ¸llerâ€“Plesset Adiabatic Connection. Journal of Physical Chemistry Letters, 2021, 12, 4867-4875. | 2.1 | 15 |
| 603 | Phonon Kinetics of Fructose at the Melting Transition. Journal of Physical Chemistry C, 2021, 125, 12269-12276. | 1.5 | 1 |
| 604 | Synergy of Solid-State NMR, Single-Crystal X-ray Diffraction, and Crystal Structure Prediction Methods: A Case Study of Teriflunomide (TFM). Crystal Growth and Design, 2021, 21, 3328-3343. | 1.4 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 605 | Kinetic resolution of racemic 6-substituted 1,2,3,4-tetrahydroquinaldines with chiral acyl chlorides. Experiment and quantum chemical simulation. Russian Chemical Bulletin, 2021, 70, 890-899. | 0.4 | 4 |
| 606 | Analysis of the relative stability of lithium halide crystal structures: Density functional theory and classical models. Journal of Chemical Physics, 2021, 154, 184507. | 1.2 | 2 |
| 607 | Vibrational spectroscopy and phononâ€related properties of monoclinic GABA, a nonâ€proteinogenic inhibitory neurotransmitter amino acid. Journal of Raman Spectroscopy, 2021, 52, 1294-1307. | 1.2 | 1 |
| 608 | Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4026-4035. | 1.1 | 31 |
| 609 | Changes in Surface Free Energy and Surface Conductivity of Carbon Nanotube/Polyimide Nanocomposite Films Induced by UV Irradiation. ACS Applied Materials & Interfaces, 2021, 13, 24218-24227. | 4.0 | 7 |
| 610 | Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€: Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie - International Edition, 2021, 60, 13144-13149. | 7.2 | 8 |
| 611 | Stability Changes in Iridium Nanoclusters via Monoxide Adsorption: A DFT Study within the van der Waals Corrections. Journal of Physical Chemistry A, 2021, 125, 4805-4818. | 1.1 | 7 |
| 612 | Energy Decomposition to Access the Stability Changes Induced by CO Adsorption on Transition-Metal 13-Atom Clusters. Journal of Chemical Information and Modeling, 2021, 61, 2294-2301. | 2.5 | 6 |
| 613 | Diffusion quantum Monte Carlo study of argon dimer. Electronic Structure, 2021, 3, 024010. | 1.0 | 1 |
| 614 | Requirements for an accurate dispersion-corrected density functional. Journal of Chemical Physics, 2021, 154, 230902. | 1.2 | 39 |
| 615 | Catalytic Asymmetric Azaâ€Dielsâ€“Alder Reaction of Ketimines and Unactivated Dienes. Angewandte Chemie, 2021, 133, 17749-17755. | 1.6 | 2 |
| 616 | Câ€“H activation. Nature Reviews Methods Primers, 2021, 1, . | 11.8 | 277 |
| 617 | Interactions between large molecules pose a puzzle for reference quantum mechanical methods. Nature Communications, 2021, 12, 3927. | 5.8 | 57 |
| 618 | Catalytic Asymmetric Azaâ€Dielsâ€“Alder Reaction of Ketimines and Unactivated Dienes. Angewandte Chemie - International Edition, 2021, 60, 17608-17614. | 7.2 | 25 |
| 619 | Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. Accounts of Chemical Research, 2021, 54, 2833-2843. | 7.6 | 21 |
| 620 | Dynamics of Ionic Liquid through Intrinsic Vibrational Probes Using the Dispersion-Corrected DFT Functionals. Journal of Physical Chemistry B, 2021, 125, 6994-7008. | 1.2 | 11 |
| 621 | The temperature - pressure phase diagram of the calcite I - calcite II phase transition: A first-principles investigation. Journal of Physics and Chemistry of Solids, 2021, 154, 110045. | 1.9 | 1 |
| 622 | Stability and Hydrogen Storage Properties of M<sub>x</sub>-B<sub>6</sub>H<sub>6</sub> Complexes (M = Yâ€“Mo, Ruâ€“Ag, x = 1â€“2). ACS Sustainable Chemistry and Engineering, 2021, 9, 10868-10881. | 3.2 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 623 | The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287. | 5.3 | 16 |
| 624 | Future directions of chemical theory and computation. Pure and Applied Chemistry, 2021, 93, 1423-1433. | 0.9 | 3 |
| 625 | Could London Dispersion Force Control Regioselective (2 + 2) Cyclodimerizations of Benzynes? YES: Application to the Synthesis of Helical Biphenylenes. Journal of the American Chemical Society, 2021, 143, 10853-10859. | 6.6 | 19 |
| 626 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801. | 1.2 | 518 |
| 627 | Three in One: The Versatility of Hydrogen Bonding Interaction in Halide Salts with Hydroxyâ€Functionalized Pyridinium Cations. ChemPhysChem, 2021, 22, 1850-1856. | 1.0 | 5 |
| 628 | Neat, Simple, and Wrong: Debunking Electrostatic Fallacies Regarding Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 7125-7137. | 1.1 | 21 |
| 629 | Computational discovery of energy materials in the era of big data and machine learning: A critical review. Materials Reports Energy, 2021, 1, 100047. | 1.7 | 24 |
| 630 | Controllable electronic effect via deep eutectic solvents modification for boosted aerobic oxidative desulfurization. Molecular Catalysis, 2021, 512, 111757. | 1.0 | 3 |
| 631 | Quantum-mechanical force balance between multipolar dispersion and Pauli repulsion in atomic van der Waals dimers. Physical Review Research, 2021, 3, . | 1.3 | 9 |
| 632 | Research of cation dependences of structural and elastic properties of metal carbonates series by density functional theory calculations. Materials Today Communications, 2021, 28, 102509. | 0.9 | 5 |
| 633 | Unified Mechanistic Concept of the Copper-Catalyzed and Amide-Oxazoline-Directed C(sp<sup>2</sup>)â€“H Bond Functionalization. ACS Catalysis, 2021, 11, 12620-12631. | 5.5 | 12 |
| 634 | Reduced-gradient analysis of van der Waals complexes. Electronic Structure, 2021, 3, 034009. | 1.0 | 7 |
| 635 | Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151. | 2.3 | 75 |
| 636 | Possible coordination modes of copper(II) atom in model silsesquioxanes complexes at various pH conditions: DFT study. Chemical Physics Letters, 2021, 778, 138739. | 1.2 | 2 |
| 637 | New computational results for a prototype of an excitable system. Results in Physics, 2021, 28, 104666. | 2.0 | 53 |
| 638 | Azideâ‹…â‹…â‹…Oxygen Interaction: A Crystal Engineering Tool for Conformational Locking. Angewandte Chemie - International Edition, 2021, 60, 22797-22803. | 7.2 | 26 |
| 639 | Azideâ‹…â‹…â‹…Oxygen Interaction: A Crystal Engineering Tool for Conformational Locking. Angewandte Chemie, 2021, 133, 22979. | 1.6 | 3 |
| 640 | Green Synthesis of Triangular ZnO Nanoparticles Using Azadirachta indica Leaf Extract and Its Shape Dependency for Significant Antimicrobial Activity: Joint Experimental and Theoretical Investigation. Journal of Cluster Science, 2022, 33, 2517-2530. | 1.7 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 641 | Predicting and Understanding Non-Covalent Interactions Using Novel Forms of Symmetry-Adapted Perturbation Theory. Accounts of Chemical Research, 2021, 54, 3679-3690. | 7.6 | 22 |
| 642 | Electric Field Induced Twisted Bilayer Graphene Infrared Plasmon Spectrum. Nanomaterials, 2021, 11, 2433. | 1.9 | 10 |
| 643 | Towards thermodynamically stable anionic dimers with â€œanti-electrostaticâ€•hydrogen bonds overcoming like-charge repulsion. Journal of Molecular Liquids, 2021, 340, 116882. | 2.3 | 2 |
| 644 | Hematite rhombuses for chemiresitive ozone sensors: Experimental and theoretical approaches. Applied Surface Science, 2021, 563, 150209. | 3.1 | 8 |
| 645 | Comparative study of halogen-doped (X Cl, Br, I) hexagonal boron nitride: A promising strategy to enhance the capacity of adsorptive desulfurization. Journal of Environmental Chemical Engineering, 2021, 9, 105886. | 3.3 | 9 |
| 646 | New models involving quantum chemical parameters for assessing the chromatographic retention process. Microchemical Journal, 2021, 170, 106693. | 2.3 | 1 |
| 647 | Diaphite-structured nanodiamonds with six- and twelve-fold symmetries. Diamond and Related Materials, 2021, 119, 108573. | 1.8 | 16 |
| 648 | Elasticity of selected icy satellite candidate materials (CO2, C6H6, MgSO4Â·7H2O and CaSO4Â·2H2O) revisited by dispersion corrected density functional theory. Icarus, 2021, 368, 114611. | 1.1 | 3 |
| 649 | Quantification and understanding of non-covalent interactions in molecular and ionic systems: Dispersion interactions and hydrogen bonding analysed by thermodynamic methods. Journal of Molecular Liquids, 2021, 343, 117547. | 2.3 | 13 |
| 650 | Solution-processed Cd-substituted CZTS nanocrystals for sensitized liquid junction solar cells. Journal of Alloys and Compounds, 2022, 890, 161575. | 2.8 | 9 |
| 651 | Three new polymorphs of 1,8-diacetylpyrene: a material with packing-dependent luminescence properties and a testbed for crystal structure prediction. Journal of Materials Chemistry C, 2021, 9, 2491-2503. | 2.7 | 6 |
| 652 | Electron confinement meet electron delocalization: non-additivity and finite-size effects in the polarizabilities and dispersion coefficients of the fullerenes. Physical Chemistry Chemical Physics, 2021, 23, 5773-5779. | 1.3 | 4 |
| 653 | Organocatalytic Enantioselective Higherâ€Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. Angewandte Chemie, 2018, 130, 1260-1264. | 1.6 | 16 |
| 654 | Effect of vacancy defects on electronic properties and wettability of coal surface. Applied Surface Science, 2020, 511, 145546. | 3.1 | 20 |
| 655 | Simulation and Assignment of the Terahertz Vibrational Spectra of Enalapril Maleate Cocrystal Polymorphs. Journal of Physical Chemistry A, 2020, 124, 9793-9800. | 1.1 | 6 |
| 656 | The Impact of Electron Correlation on Describing QM/MM Interactions in the Attendant Molecular Dynamics Simulations of CO in Myoglobin. Scientific Reports, 2020, 10, 8539. | 1.6 | 6 |
| 657 | Noncovalent Interactions in Key Metal-centred Catalytic Intermediates: Structureâ€“Electronic Relationship. RSC Catalysis Series, 2019, , 579-607. | 0.1 | 1 |
| 658 | Vibrations of the guanineâ€“cytosine pair in chloroform: an anharmonic computational study. Physical Chemistry Chemical Physics, 2020, 22, 5509-5522. | 1.3 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 659 | Overcoming the difficulties of predicting conformational polymorph energetics in molecular crystals via correlated wavefunction methods. Chemical Science, 2020, 11, 2200-2214. | 3.7 | 48 |
| 660 | Thermal expansion in dispersion-bound molecular crystals. Physical Review Materials, 2018, 2, . | 0.9 | 18 |
| 661 | Nonlocal van der Waals functionals for solids: Choosing an appropriate one. Physical Review Materials, 2019, 3, . | 0.9 | 65 |
| 662 | Benchmarking van der Waals-treated DFT: The case of hexagonal boron nitride and graphene on Ir(111). Physical Review Materials, 2019, 3, . | 0.9 | 12 |
| 663 | Prediction of Li intercalation voltages in rechargeable battery cathode materials: Effects of exchange-correlation functional, van der Waals interactions, and Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>. Physical Review Materials, 2020, 4, . | 0.9 | 15 |
| 664 | Ab initio investigation of the role of charge transfer in the adsorption properties of H2,ÂN2,ÂO2,CO,NO,CO2,ÂNO2 , and CH4 on the van der Waals layered Sn3O4 semiconductor. Physical Review Materials, 2020, 4, . | 0.9 | 1 |
| 665 | Quantum chemical exercise linking computational chemistry to general chemistry topics. Chemistry Teacher International, 2021, 3, . | 0.9 | 5 |
| 666 | DFT Study of the Mechanisms of Transition-Metal-Catalyzed Reductive Coupling Reactions. Current Organic Chemistry, 2020, 24, 1367-1383. | 0.9 | 5 |
| 667 | Chiral analysis of pantolactone with molecular rotational resonance spectroscopy. Chirality, 2022, 34, 114-125. | 1.3 | 17 |
| 668 | Adsorption energies of porphyrins on MgO(100): An experimental benchmark for dispersion-corrected density-functional theory. Surface Science, 2022, 717, 121979. | 0.8 | 7 |
| 669 | Unraveling the effects of O-doping into h-BN on the adsorptive desulfurization performance by DFT calculations. Journal of Environmental Chemical Engineering, 2021, 9, 106463. | 3.3 | 17 |
| 670 | Molecular adsorption of iminotriazine derivatives on graphene. JPhys Materials, 2020, 3, 034011. | 1.8 | 4 |
| 672 | 0D Bismuth(III)-Based Hybrid Ferroelectric: Tris(acetamidinium) Hexabromobismuthate(III). Chemistry of Materials, 2021, 33, 8591-8601. | 3.2 | 22 |
| 673 | Excitedâ€State Dynamics of a metaâ€Dimethylamino Locked GFP Chromophore as a Fluorescence Turnâ€on Water Sensor<sup>â€</sup>. Photochemistry and Photobiology, 2022, 98, 311-324. | 1.3 | 4 |
| 674 | Structure-Property Relationships of Polymers, Unraveled by Molecular Orbital, RIS, and Periodic Density Functional Theory Calculations. ACS Symposium Series, 2020, , 161-208. | 0.5 | 1 |
| 675 | Structure and Photophysical Properties of 1,1,2,2â€Tetra(1â€anthryl)ethane: A C(sp3)â€“C(sp3) Bond Substituted with Four Anthracene Units. ChemPlusChem, 2021, , . | 1.3 | 2 |
| 676 | Exploring the Properties of H 2 O@C 60 with the Local Secondâ€Order MÃ¸llerâ€Plesset Perturbation Theory: Blue or Red Shift in C 60 and H 2 O Fundamentals to Expect?. ChemistrySelect, 2021, 6, 11583-11590. | 0.7 | 2 |
| 677 | Adsorption of CH4 on the Pt(111) surface: Random phase approximation compared to density functional theory. Journal of Chemical Physics, 2021, 155, 174702. | 1.2 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 678 | The Cyclization of Allenylâ€Substituted Hydroxylamines to 1,2â€Oxazines: an Experimental and Computational Study. European Journal of Organic Chemistry, 2020, 2020, 6740-6748. | 1.2 | 1 |
| 679 | Exhibiting environment sensitive optical properties through multiscale modelling: A study of photoactivatable probes. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 425, 113672. | 2.0 | 2 |
| 680 | Real-space imaging of anisotropic charge of ï*f*-hole by means of Kelvin probe force microscopy. Science, 2021, 374, 863-867. | 6.0 | 71 |
| 681 | Enabling Large-Scale Condensed-Phase Hybrid Density Functional Theory-Based Ab Initio Molecular Dynamics II: Extensions to the Isobaricâ€“Isoenthalpic and Isobaricâ€“Isothermal Ensembles. Journal of Chemical Theory and Computation, 2021, 17, 7789-7813. | 2.3 | 7 |
| 682 | Assessment of the van der Waals, Hubbard U parameter and <scp>spinâ€orbit</scp> coupling corrections on the <scp>2D</scp>/<scp>3D</scp> structures from metal gold congeners clusters. Journal of Computational Chemistry, 2022, 43, 230-243. | 1.5 | 4 |
| 683 | London Dispersion Helps Refine Steric A-Values: Dispersion Energy Donor Scales. Journal of the American Chemical Society, 2021, 143, 20837-20848. | 6.6 | 35 |
| 684 | Enhancing the Accuracy of Ab Initio Molecular Dynamics by Fine Tuning of Effective Two-Body Interactions: Acetonitrile as a Test Case. Journal of Physical Chemistry A, 2021, 125, 10475-10484. | 1.1 | 4 |
| 685 | Electron spin resonance of single iron phthalocyanine molecules and role of their non-localized spins in magnetic interactions. Nature Chemistry, 2022, 14, 59-65. | 6.6 | 51 |
| 686 | Static and dynamic water structures at interfaces: A case study with focus on Pt(111). Journal of Chemical Physics, 2021, 155, 194702. | 1.2 | 3 |
| 687 | Synthesis, Structures, and Properties of Helically Fused Anthraquinones with Unusually Close Carbonylâ€Carbonyl Contacts. Chemistry - A European Journal, 2021, , . | 1.7 | 3 |
| 688 | Coming of Age of Computational Chemistry from a Resilient Past to a Promising Future. Israel Journal of Chemistry, 0, , . | 1.0 | 2 |
| 689 | Correlation Effects in Trimeric Acylphloroglucinols. Computation, 2021, 9, 121. | 1.0 | 5 |
| 690 | Comparative study of the effect of van der Waals interactions on stacking fault energies in SiC. Journal of Applied Physics, 2021, 130, . | 1.1 | 3 |
| 691 | Theoretical Approach to Evaluate the Gas-Sensing Performance of Graphene Nanoribbon/Oligothiophene Composites. ACS Omega, 2022, 7, 2260-2274. | 1.6 | 6 |
| 692 | Tunnelling assisted hydrogen elimination mechanisms of FeCl3/TEMPO. Chemical Communications, 2022, 58, 565-568. | 2.2 | 5 |
| 693 | Performance comparison of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>r</mml:mi></mml:mrow><mml:mn>2</mml:mn> and SCAN metaGGA density functionals for solid materials via an automated, high-throughput computational workflow. Physical Review Materials, 2022, 6, . | 0.9 | 31 |
| 694 | Coronene surface for delivery of Favipiravir: Computational approach. Inorganic Chemistry Communication, 2022, 136, 109133. | 1.8 | 3 |
| 695 | 2D IR spectra of the intrinsic vibrational probes of ionic liquid from dispersion corrected DFT-MD simulations. Journal of Molecular Liquids, 2022, 348, 118390. | 2.3 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 696 | Theoretical studies on cycloaddition reactions of N-allyl substituted polycyclic Isoindole-1,3-dione with nitrones and nitrile oxides. Computational and Theoretical Chemistry, 2022, 1208, 113574. | 1.1 | 10 |
| 697 | Structure of PtRu/Ru(0Â0Â0Â1) and AgPd/Pd(1Â1Â1) surface alloys: A kinetic Monte Carlo study. Chemical Physics, 2022, 555, 111428. | 0.9 | 4 |
| 698 | Impurity Controlled near Infrared Surface Plasmonic in AlN. Nanomaterials, 2022, 12, 459. | 1.9 | 1 |
| 699 | Correlation between the Stability of Substituted Cobaltocenium and Molecular Descriptors. Journal of Physical Chemistry A, 2022, 126, 80-87. | 1.1 | 5 |
| 700 | Structural Properties and Magnetic Ground States of 100 Binary d-Metal Oxides Studied by Hybrid Density Functional Methods. Molecules, 2022, 27, 874. | 1.7 | 13 |
| 701 | How many more polymorphs of ROY remain undiscovered. Chemical Science, 2022, 13, 1288-1297. | 3.7 | 41 |
| 702 | Ab Initio Simulations of Water/Metal Interfaces. Chemical Reviews, 2022, 122, 10746-10776. | 23.0 | 72 |
| 703 | Polymorphism and optical, magnetic and thermal properties of the either phyllo- or inosilicate-analogous borosulfate Cu[B<sub>2</sub>(SO<sub>4</sub>)<sub>4</sub>]. Dalton Transactions, 2022, 51, 3104-3115. | 1.6 | 5 |
| 704 | Theoretical study of hydrogen adsorption on the graphene quantum dots doped with various first row transition metals: Switch of spin state as a way to improve H2 adsorption. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 139, 115144. | 1.3 | 8 |
| 705 | Half antiperovskites VII â€“ DFT modelling of shandites that are isoelectronic to Co 3 Sn 2 S 2. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , . | 0.6 | 1 |
| 706 | Thermodynamically Stable Cationic Dimers in Carboxyl-Functionalized Ionic Liquids: The Paradoxical Case of â€œAnti-Electrostaticâ€•Hydrogen Bonding. Molecules, 2022, 27, 366. | 1.7 | 0 |
| 707 | A contribution of molecular modeling to supramolecular structures in soil organic matter<sup>#</sup>. Journal of Plant Nutrition and Soil Science, 2022, 185, 44-59. | 1.1 | 14 |
| 708 | Quantum framework for describing retarded and nonretarded molecular interactions in external electric fields. Physical Review Research, 2022, 4, . | 1.3 | 11 |
| 709 | Speciation of organoarsenicals in aqueous solutions by Raman spectrometry and quantum chemical calculations. Microchemical Journal, 2022, 175, 107186. | 2.3 | 2 |
| 710 | Properties of binary mixtures of a novel natural deep eutectic solvent (glycolic acidÂ+Âxylitol) and water at several temperatures. Fluid Phase Equilibria, 2022, 556, 113390. | 1.4 | 4 |
| 711 | Theoretical studies on molecular conformers and infrared spectra of Triethylamine. Wuli Xuebao/Acta Physica Sinica, 2022, . | 0.2 | 0 |
| 712 | Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies. Chemical Reviews, 2022, 122, 6117-6321. | 23.0 | 195 |
| 713 | Behavior of counterpoise correction in manyâ€body molecular clusters of organic compounds: <scp>Hartreeâ€“Fock</scp> interaction energy perspective. Journal of Computational Chemistry, 2022, 43, 568-576. | 1.5 | 5 |

| # | Article | IF | Citations |
|---|---|---|---|
| 714 | Evaluating Hydrogen Bonding in Organic Cocrystals Using Low-Frequency Raman Vibrational Spectroscopy and Quantum Mechanical Simulations. Crystal Growth and Design, 2022, 22, 1922-1932. | 1.4 | 5 |
| 715 | O(N) Stochastic Evaluation of Many-Body van der Waals Energies in Large Complex Systems. Journal of Chemical Theory and Computation, 2022, 18, 1633-1645. | 2.3 | 12 |
| 716 | Amphiphilic cyclodextrins: Dimerization and diazepam binding explored by molecular dynamics simulations. Journal of Molecular Liquids, 2022, 349, 118457. | 2.3 | 6 |
| 717 | Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161. | 1.4 | 9 |
| 718 | A first-principles study of water adsorbed on flat and stepped silver surfaces. Physical Chemistry Chemical Physics, 2022, 24, 6803-6810. | 1.3 | 4 |
| 720 | On the mechanism of electrochemical functionalization of carbon nanotubes with different structures with aminophenylphosphonic acid isomers: an experimental and computational approach. Journal of Materials Chemistry A, 2022, 10, 7271-7290. | 5.2 | 4 |
| 721 | Computational Chemistry as a Conceptual Game Changer: Understanding the Role of London Dispersion in Hexaphenylethane Derivatives (Gomberg Systems). Israel Journal of Chemistry, 2022, 62, . | 1.0 | 12 |
| 722 | Frustrated and Realized Hydrogen Bonding in 4-Hydroxy-3,5-ditertbutylphenylphosphine Derivatives. Crystal Growth and Design, 2022, 22, 2512-2533. | 1.4 | 8 |
| 723 | QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524. | 2.5 | 6 |
| 724 | Appraisal of dispersion damping functions for the effective fragment potential method. Molecular Physics, 2023, 121, . | 0.8 | 0 |
| 725 | The PM6-FGC Method: Improved Corrections for Amines and Amides. Molecules, 2022, 27, 1678. | 1.7 | 2 |
| 726 | Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs. Journal of Physical Chemistry C, 2022, 126, 6000-6007. | 1.5 | 6 |
| 727 | All-hydrocarbon, all-conjugated cycloparaphenylene-polycyclic aromatic hydrocarbon host-guest complexes stabilized by CHâ‹¯Ï€ interactions. Nano Research, 2022, 15, 5545-5555. | 5.8 | 11 |
| 728 | Challenges with Simulating Modified RNA: Insights into Role and Reciprocity of Experimental and Computational Approaches. Genes, 2022, 13, 540. | 1.0 | 4 |
| 729 | Vibrational Modes and Terahertz Phenomena of the Large-Cage Zeolitic Imidazolate Framework-71. Journal of Physical Chemistry Letters, 2022, 13, 2838-2844. | 2.1 | 11 |
| 730 | Computational Evaluation and Design of Polyethylene Zirconocene Catalysts with Noncovalent Dispersion Interactions. Organometallics, 2022, 41, 581-593. | 1.1 | 4 |
| 731 | Lateral Interactions of Dynamic Adlayer Structures from Artificial Neural Networks. Journal of Physical Chemistry C, 2022, 126, 5529-5540. | 1.5 | 5 |
| 732 | Highâ€Temperature Quantum Tunneling and Hydrogen Bonding Rearrangements Characterize the Solidâ€Solid Phase Transitions in a Phosphoniumâ€Based Protic Ionic Liquid. Chemistry - A European Journal, 2022, , . | 1.7 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 733 | Microscopic EDL structures and chargeâ€“potential relation on stepped platinum surface: Insights from the ab initio molecular dynamics simulations. Journal of Chemical Physics, 2022, 156, 104701. | 1.2 | 12 |
| 734 | Adsorption of Transition-Metal Clusters on Graphene and N-Doped Graphene: A DFT Study. Langmuir, 2022, 38, 3694-3710. | 1.6 | 23 |
| 735 | Assessing the persistence of chalcogen bonds in solution with neural network potentials. Journal of Chemical Physics, 2022, 156, 154112. | 1.2 | 6 |
| 736 | Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. Journal of Chemical Physics, 2022, 156, 134105. | 1.2 | 32 |
| 737 | Bonding character of intermediates in onâ€surface Ullmann reactions revealed with energy decomposition analysis. Journal of Computational Chemistry, 2023, 44, 179-189. | 1.5 | 2 |
| 738 | A rare diiodo-L-tyrosine copper(II) complexes â€“ Crystal and molecular structure of materials stabilized by weak interactions. Polyhedron, 2022, 219, 115780. | 1.0 | 0 |
| 739 | Electronic Energy and Local Property Errors at QTAIM Critical Points while Climbing Perdewâ€™s Ladder of Density-Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 293-308. | 2.3 | 14 |
| 740 | Kinetically Controlled Reduction of Î²-Vanadyl(V) Orthophosphate: Synthesis and Characterization of New Metastable Polymorphs of Vanadium(III) Phosphate. Inorganic Chemistry, 2022, 61, 507-519. | 1.9 | 0 |
| 741 | Implicit Solvation Methods for Catalysis at Electrified Interfaces. Chemical Reviews, 2022, 122, 10777-10820. | 23.0 | 82 |
| 742 | Electron Correlation: Nature's Weird and Wonderful Chemical Glue. Israel Journal of Chemistry, 2022, 62, . | 1.0 | 13 |
| 743 | An open-source framework for fast-yet-accurate calculation of quantum mechanical features. Physical Chemistry Chemical Physics, 2022, , . | 1.3 | 1 |
| 744 | Catalyst sites and active species in the early stages of MTO conversion over cobalt AlPO-18 followed by IR spectroscopy. Catalysis Science and Technology, 2022, 12, 2775-2792. | 2.1 | 8 |
| 745 | Conformational characteristics and conformation-dependent properties of poly(Îµ-caprolactone). Physical Chemistry Chemical Physics, 2022, , . | 1.3 | 3 |
| 746 | Open-Shell Variant of the London Dispersion-Corrected Hartreeâ€“Fock Method (HFLD) for the Quantification and Analysis of Noncovalent Interaction Energies. Journal of Chemical Theory and Computation, 2022, 18, 2292-2307. | 2.3 | 7 |
| 747 | First-Principle Studies of the Structural, Electronic, Mechanical, and Vibrational Properties of Double Carbonates with a Dolomite Structure. Izvestiya of Altai State University, 2022, , 23-29. | 0.1 | 0 |
| 748 | Photocatalytic Degradation of Rhodamine B Dye and Hydrogen Evolution by Hydrothermally Synthesized NaBH4â€”Spiked ZnS Nanostructures. Frontiers in Chemistry, 2022, 10, 835832. | 1.8 | 10 |
| 749 | Beyond Steric Crowding: Dispersion Energy Donor Effects in Large Hydrocarbon Ligands. Accounts of Chemical Research, 2022, 55, 1337-1348. | 7.6 | 25 |
| 750 | Tracing the Primordial Chemical Life of Glycine: A Review from Quantum Chemical Simulations. International Journal of Molecular Sciences, 2022, 23, 4252. | 1.8 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 751 | External electric field to control the Dielsâ€“Alder reactions of endohedral fullerene. Physical Chemistry Chemical Physics, 2022, 24, 11131-11136. | 1.3 | 4 |
| 752 | Noncovalently bound excited-state dimers: a perspective on current time-dependent density functional theory approaches applied to aromatic excimer models. RSC Advances, 2022, 12, 13014-13034. | 1.7 | 18 |
| 753 | TAO-DFT fictitious temperature made simple. RSC Advances, 2022, 12, 12193-12210. | 1.7 | 7 |
| 754 | Chiral Analysis of Linalool, an Important Natural Fragrance and Flavor Compound, by Molecular Rotational Resonance Spectroscopy. Symmetry, 2022, 14, 917. | 1.1 | 7 |
| 755 | First-Principles Investigation of Electronic Properties and Phase Transition of Ti<sub>3</sub>O<sub>5</sub>. Journal of Physical Chemistry C, 2022, 126, 7809-7817. | 1.5 | 8 |
| 756 | Accurate Deep Learning-Aided Density-Free Strategy for Many-Body Dispersion-Corrected Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 4381-4388. | 2.1 | 12 |
| 757 | Probing the SO<sub>2</sub>Adsorption Mechanism in Hofmann Clathrates via Inelastic Neutron Scattering and Density Functional Theory Calculations. Journal of Physical Chemistry C, 2022, 126, 8090-8099. | 1.5 | 7 |
| 758 | Study on Hydration and Dehydration of Ezetimibe by Terahertz Spectroscopy with Humidity-Controlled Measurements and Theoretical Analysis. Journal of Physical Chemistry A, 2022, 126, 2879-2888. | 1.1 | 3 |
| 759 | Development and testing of an algorithm for efficient MP2/CCSD(T) energy estimation of molecular clusters with the 2â€“body approach. Journal of Computational Chemistry, 2022, , . | 1.5 | 0 |
| 760 | Increasing Complexity in a Conformer Space Step-by-Step: Weighing London Dispersion against Cationâˆ’Ï€ Interactions. Journal of the American Chemical Society, 2022, 144, 9007-9022. | 6.6 | 13 |
| 761 | First-principle studies of electronic, elastic and vibrational properties of barytocalcite and paralstonite. Materials Today Communications, 2022, 31, 103644. | 0.9 | 0 |
| 762 | Dispersion Interactions in Exciton-Localized States. Theory and Applications to Ïâ€“Ï€* and nâˆ’Ï€* Excited States. Journal of Chemical Theory and Computation, 2022, 18, 3497-3511. | 2.3 | 4 |
| 764 | Can Domain-Based Local Pair Natural Orbitals Approaches Accurately Predict Phosphorescence Energies?. Physical Chemistry Chemical Physics, 0, , . | 1.3 | 3 |
| 765 | Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535. | 1.1 | 16 |
| 766 | P-functionalized carbon nanotubes promote highly stable electrocatalysts based on Fe-phthalocyanines for oxygen reduction: Experimental and computational studies. Journal of Energy Chemistry, 2022, 72, 276-290. | 7.1 | 11 |
| 767 | In Situ Observation of the Structure of Crystallizing Magnesium Sulfate Heptahydrate Solutions with Terahertz Transmission Spectroscopy. Crystal Growth and Design, 0, , . | 1.4 | 1 |
| 768 | Spirooxazine-Based Dual-Sensing Probe for Colorimetric Detection of Cu<sup>2+</sup> and Fe<sup>3+</sup> and Its Application in Drinking Water and Rice Quality Monitoring. ACS Omega, 2022, 7, 18671-18680. | 1.6 | 12 |
| 769 | The contribution of intermolecular spin interactions to the London dispersion forces between chiral molecules. Journal of Chemical Physics, 2022, 156, . | 1.2 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 770 | Optimization of the r<sup>2</sup>SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2022, 126, 3826-3838. | 1.1 | 8 |
| 771 | Tailoring Multifunctional Small Molecular Photosensitizers to In Vivo Selfâ€Assemble with Albumin to Boost Tumorâ€Preferential Accumulation, NIR Imaging, and Photodynamic/Photothermal/Immunotherapy. Small, 2022, 18, . | 5.2 | 11 |
| 772 | Rational Computational Design of Systems Exhibiting Strong Halogen Bonding Involving Fluorine in Bicyclic Diamine Derivatives. Journal of Organic Chemistry, 2022, 87, 8413-8419. | 1.7 | 2 |
| 773 | On the stability of MOPO4 structure types with M: V, Mo, Nb, W, Ta, Sb. Journal of Solid State Chemistry, 2022, 312, 123221. | 1.4 | 0 |
| 775 | Simulating the solvation structure of low- and high-spin [Fe(bpy)<sub>3</sub>]<sup>2+</sup>: long-range dispersion and many-body effects. Physical Chemistry Chemical Physics, 2022, 24, 16655-16670. | 1.3 | 3 |
| 776 | Charge Carrier Management in Semiconductors: Modeling Charge Transport and Recombination. Springer Handbooks, 2022, , 365-398. | 0.3 | 2 |
| 777 | Long-range dispersion-inclusive machine learning potentials for structure search and optimization of hybrid organicâ€“inorganic interfaces. , 2022, 1, 463-475. | | 16 |
| 778 | Spectroscopic evidence of Sâ‹¯N and Sâ‹¯O hemibonds in heterodimer cations. Physical Chemistry Chemical Physics, 2022, 24, 19354-19361. | 1.3 | 5 |
| 779 | Stabilization of Glucosyl Dioxolenium Ions by â€œDual Participationâ€• of the 2,2-Dimethyl-2-(ortho-nitrophenyl)acetyl (DMNPA) Protection Group for 1,2-cis-Glucosylation. Journal of Organic Chemistry, 2022, 87, 9139-9147. | 1.7 | 11 |
| 780 | Efficient and Accurate Description of Dielsâ€Alder Reactions Using Density Functional Theory**. ChemPhysChem, 2022, 23, . | 1.0 | 6 |
| 781 | Ag Atom Anchored on Defective Hexagonal Boron Nitride Nanosheets As Single Atom Adsorbents for Enhanced Adsorptive Desulfurization via S-Ag Bonds. Nanomaterials, 2022, 12, 2046. | 1.9 | 11 |
| 783 | Surface Reactivity of Cementitious Crystals Alite and Belite. Journal of Physical Chemistry C, 2022, 126, 11265-11276. | 1.5 | 0 |
| 784 | Complete Set of Diketopyrrolopyrrole Centrosymmetrical Cofacial Stacked Pairs. ChemPhysChem, 2022, 23, . | 1.0 | 6 |
| 785 | Coupled Cluster Benchmarking of Large Noncovalent Complexes in L7 and S12L as Well as the C<sub>60</sub> Dimer, DNAâ€“Ellipticine, and HIVâ€“Indinavir. Journal of Physical Chemistry A, 2022, 126, 4326-4341. | 1.1 | 11 |
| 786 | Theoretical study of the stereoselectivity in the reaction of 4-haloglutamic acid derivatives with arylamines. Russian Chemical Bulletin, 2022, 71, 1135-1142. | 0.4 | 2 |
| 787 | Combining micro-infrared reflection absorption spectroscopy with density functional theory for investigating the adsorption of organic friction modifiers on steel surfaces. Vibrational Spectroscopy, 2022, 121, 103403. | 1.2 | 1 |
| 788 | Substitution Effects on the Reactivity and Thermostability of Five-Membered Ring Fluorides. ACS Omega, 2022, 7, 25476-25490. | 1.6 | 2 |
| 789 | Dissecting Noncovalent Interactions in Carboxylâ€Functionalized Ionic Liquids Exhibiting Double and Single Hydrogens Bonds Between Ions of Like Charge. Chemistry - A European Journal, 2022, 28, . | 1.7 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 790 | Accurate Determination of Adsorption-Energy Differences of Metalloporphyrins on Rutile TiO<sub>2</sub>(110) 1 Ã— 1. Langmuir, 2022, 38, 8643-8650. | 1.6 | 1 |
| 791 | A litmus test for the balanced description of dispersion interactions and coordination chemistry of lanthanoids. Physical Chemistry Chemical Physics, 0, , . | 1.3 | 1 |
| 792 | Ionic Dynamics and Vibrational Spectral Diffusion of a Protic Alkylammonium Ionic Salt through Intrinsic Cationic Nâ€“H Vibrational Probe from FPMD Simulations. Journal of Physical Chemistry A, 2022, 126, 5134-5147. | 1.1 | 1 |
| 793 | Feasible Cluster Model Method for Simulating the Redox Potentials of Laccase CueO and Its Variant. Frontiers in Bioengineering and Biotechnology, 0, 10, . | 2.0 | 1 |
| 794 | Tailoring the hydrogen storage performance of the Cr-, Mn-, and Fe-doped circumcoronenes by the presence of N and B co-dopants: Computational study. International Journal of Hydrogen Energy, 2022, 47, 34570-34582. | 3.8 | 3 |
| 795 | Nanoscale MXene Interlayer and Substrate Adhesion for Lubrication: A Density Functional Theory Study. ACS Applied Nano Materials, 2022, 5, 10516-10527. | 2.4 | 28 |
| 796 | Binding propensity and selectivity of cationic, anionic, and neutral guests with model hydrophobic hosts: A first principles study. Journal of Computational Chemistry, 2023, 44, 432-441. | 1.5 | 3 |
| 797 | Low-Frequency Vibrational Spectroscopy and Quantum Mechanical Simulations of the Crystalline Polymorphs of the Antiviral Drug Ribavirin. Molecular Pharmaceutics, 2022, 19, 3385-3393. | 2.3 | 6 |
| 798 | Beyond GGA total energies for solids and surfaces. Journal of Chemical Physics, 2022, 157, 050401. | 1.2 | 1 |
| 799 | Modeling of Structure H Carbon Dioxide Clathrate Hydrates: Guestâ€“Lattice Energies, Crystal Structure, and Pressure Dependencies. Journal of Physical Chemistry C, 2022, 126, 14832-14842. | 1.5 | 4 |
| 800 | Verification of the Accuracy and Efficiency of Dispersion-Corrected Density Functional Theory Methods to Describe the Lattice Structure and Energy of Energetic Cocrystals. Crystal Growth and Design, 2022, 22, 5307-5321. | 1.4 | 5 |
| 801 | Quantum computational quantification of proteinâ€“ligand interactions. International Journal of Quantum Chemistry, 2022, 122, . | 1.0 | 27 |
| 802 | Comment on â€œRevealing the new structure of B8N8 nanocage and comparison of hydrogen storage capacityâ€•[Chem. Phys. 559 (2022) 111540]. Chemical Physics, 2022, 562, 111673. | 0.9 | 0 |
| 803 | Copigmentation effect of flavonols on anthocyanins in black mulberry juice and their interaction mechanism investigation. Food Chemistry, 2023, 399, 133927. | 4.2 | 8 |
| 804 | Semiempirical quantum mechanical methods. , 2023, , 67-92. | | 1 |
| 805 | Density-functional theory. , 2023, , 27-65. | | 0 |
| 806 | Ethynylene-linked multifunctional benzoxazines: the effect of the ethynylene group and packing on thermal behavior. Polymer Chemistry, 2022, 13, 5590-5596. | 1.9 | 5 |
| 807 | Redox-switchable hostâ€“guest complexes of metallocenes and [8]cycloparaphenylene. Nanoscale, 2022, 14, 14276-14285. | 2.8 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 808 | Intramolecular Hydrogen Bonding Patterns and Conformational Preferences of Ouabainâ€"A Molecule with Cardiotonic and Antiviral Activities. Engineering Materials, 2022, , 671-696. | 0.3 | 0 |
| 809 | DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. Physical Chemistry Chemical Physics, 2022, 24, 28700-28781. | 1.3 | 91 |
| 810 | Hidden ordered structure in the archetypical Fe(pyrazine)[Pt(CN)<sub>4</sub>] spin-crossover porous coordination compound. CrystEngComm, 2022, 24, 6349-6356. | 1.3 | 6 |
| 811 | A flexible and scalable scheme for mixing computed formation energies from different levels of theory. Npj Computational Materials, 2022, 8, . | 3.5 | 8 |
| 812 | How van der Waals Approximation Methods Affect Activation Barriers of Cyclohexene Hydrogenation over a Pd Surface. ACS Engineering Au, 0, , . | 2.3 | 0 |
| 813 | Photochemical Dearomative Cycloadditions of Quinolines and Alkenes: Scope and Mechanism Studies. Journal of the American Chemical Society, 2022, 144, 17680-17691. | 6.6 | 31 |
| 814 | Biological activity of some thiazolylâ€thiadiazines as BACEâ€1 inhibitors for Alzheimer's disease in the light of density functional theory based quantum descriptors. Journal of Physical Organic Chemistry, 2023, 36, . | 0.9 | 0 |
| 815 | Bestâ€Practice DFT Protocols for Basic Molecular Computational Chemistry**. Angewandte Chemie, 2022, 134, . | 1.6 | 36 |
| 816 | Bestâ€Practice DFT Protocols for Basic Molecular Computational Chemistry**. Angewandte Chemie - International Edition, 2022, 61, . | 7.2 | 168 |
| 817 | Bromine Pentafluoride BrF<sub>5</sub>, the Formation of [BrF<sub>6</sub>]<sup>â^'</sup> Salts, and the Stereochemical (In)activity of the Bromine Lone Pairs. Chemistry - A European Journal, 2022, 28, . | 1.7 | 7 |
| 818 | First-Principles Calculations to Investigate the Effect of Van der Waals Interactions on the Crystal and Electronic Structures of Tin-Based 0D Hybrid Perovskites. Inorganics, 2022, 10, 155. | 1.2 | 25 |
| 819 | The Stacking Faulted Nature of the Narrow Gap Semiconductor Sc2Si2Te6. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , . | 0.6 | 1 |
| 820 | Role of van der Waals interactions on the binding energies of 2D transition-metal dichalcogenides. Applied Surface Science, 2023, 608, 155163. | 3.1 | 13 |
| 821 | Structures of the (Imidazole)nH+ ... Ar (n=1,2,3) complexes determined from IR spectroscopy and quantum chemical calculations. Structural Chemistry, 2023, 34, 203-213. | 1.0 | 1 |
| 822 | Chalcogen controlled redox behaviour in peri-substituted S, Se and Te naphthalene derivatives. New Journal of Chemistry, 0, , . | 1.4 | 2 |
| 823 | Systematic Evaluation of Counterpoise Correction in Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 6742-6756. | 2.3 | 20 |
| 824 | Chemical Bonding Effects and Physical Properties of Noncentrosymmetric Hexagonal Fluorocarbonates ABCO3F (A: K, Rb, Cs; B: Mg, Ca, Sr, Zn, Cd). Molecules, 2022, 27, 6840. | 1.7 | 3 |
| 825 | Density functional theory demonstrates orientation effects in the Raman spectra of hydroxyâ€and carbonated apatite. Journal of Raman Spectroscopy, 2023, 54, 159-170. | 1.2 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 826 | In Situ Kinetic Studies of Rh(II)-Catalyzed Câ€“H Functionalization to Achieve High Catalyst Turnover Numbers. ACS Catalysis, 2022, 12, 13400-13410. | 5.5 | 6 |
| 827 | Theoretical Study of the Effect of Pressure on the Structure and Electronic Properties of Metal Carbonates. Bulletin of the Russian Academy of Sciences: Physics, 2022, 86, 1230-1241. | 0.1 | 0 |
| 828 | Effect of the Silicaâ€“Magnetite Nanocomposite Coating Functionalization on the Doxorubicin Sorption/Desorption. Pharmaceutics, 2022, 14, 2271. | 2.0 | 7 |
| 829 | Insights of hydrogen adsorption and dissociation on Ni doped Mg4 clusters: A DFT study. Computational and Theoretical Chemistry, 2022, 1217, 113907. | 1.1 | 5 |
| 830 | How to Stabilize Carbenes in Enzyme Active Sites without Metal Ions. Journal of the American Chemical Society, 2022, 144, 20739-20751. | 6.6 | 5 |
| 831 | Seeking widely applicable dispersion-corrected GGA functionals: The performances of TCA+D3 and RevTCA+D3 on solid-state systems. Computational Materials Science, 2023, 216, 111826. | 1.4 | 1 |
| 832 | Deep eutectic solvents with multiple catalytic sites for highly efficient extractive and oxidative desulfurization. Fuel, 2023, 333, 126329. | 3.4 | 8 |
| 833 | Barrier heights, reaction energies and bond dissociation energies for RH + HO<sub>2</sub>reactions with coupled-cluster theory, density functional theory and diffusion quantum Monte Carlo methods. Physical Chemistry Chemical Physics, 2022, 25, 341-350. | 1.3 | 2 |
| 834 | Native defects in monolayer GaS and GaSe: Electrical properties and thermodynamic stability. Physical Review Materials, 2022, 6, . | 0.9 | 2 |
| 835 | Electrochemical CO2 reduction: From catalysts to reactive thermodynamics and kinetics. Carbon Capture Science & Technology, 2023, 6, 100081. | 4.9 | 8 |
| 836 | The hydrogen storage capacities of 4d transition metals in various boron systems. Journal of Energy Storage, 2023, 57, 106216. | 3.9 | 3 |
| 837 | Sodium complexes as precise tools for cutting polymer chains. Exploration of PLA degradation by unique cooperation of sodium centers. Inorganic Chemistry Frontiers, 2023, 10, 1076-1090. | 3.0 | 2 |
| 838 | Towards predictive computational catalysis â€“ a case study of olefin metathesis with Mo imido alkylidene N-heterocyclic carbene catalysts. Chemical Modelling, 2022, , 1-23. | 0.2 | 1 |
| 839 | DFT calculations in solution systems: solvation energy, dispersion energy and entropy. Physical Chemistry Chemical Physics, 2023, 25, 913-931. | 1.3 | 14 |
| 840 | Physical image of amino acid interaction on graphene surface: Scientific fundamental for biological identification and detection from first-principles. Diamond and Related Materials, 2023, 131, 109571. | 1.8 | 2 |
| 841 | A theoretical framework for the design of molecular crystal engines. Chemical Science, 2023, 14, 937-949. | 3.7 | 7 |
| 842 | A benchmark for non-covalent interactions in organometallic crystals. Physical Chemistry Chemical Physics, 2022, 24, 29338-29349. | 1.3 | 0 |
| 843 | Ab Initio Studies of the Influence of Pressure on the Structure and Electronic and Elastic Properties of Carbonates of Alkaline and Alkaline-Earth Metals. Physics of the Solid State, 2022, 64, 405-415. | 0.2 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 844 | Multiscale Computational Approaches toward the Understanding of Materials. Advanced Theory and Simulations, 2023, 6, . | 1.3 | 4 |
| 845 | Semisynthetic Approach toward Biologically Active Derivatives of Phenylspirodrimanes from S. chartarum. ACS Omega, 2022, 7, 45215-45230. | 1.6 | 3 |
| 846 | Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. Journal of Chemical Theory and Computation, 2022, 18, 7166-7178. | 2.3 | 2 |
| 847 | Efficient Computation of the Interaction Energies of Very Large Non-covalently Bound Complexes. Synlett, 2023, 34, 1135-1146. | 1.0 | 2 |
| 848 | Mechanistic Details of the Pdâ€catalyzed and MPAA Ligandâ€Enabled Î²â€C(sp3)â€H Acetoxylation of Free Carboxylic Acid. Chemistry - an Asian Journal, 0, , . | 1.7 | 0 |
| 849 | Thermochemical evaluation of adaptive and fixed density functional theory quadrature schemes. Journal of Chemical Physics, 2022, 157, 234106. | 1.2 | 0 |
| 850 | Mind the Interface Gap: Exposing Hidden Interface Defects at the Epitaxial Heterostructure between CuO and Cu<sub>2</sub>O. ACS Applied Materials & Interfaces, 2022, 14, 56331-56343. | 4.0 | 1 |
| 851 | Modeling of BN-Doped Carbon Nanotube as High-Performance Thermoelectric Materials. Nanomaterials, 2022, 12, 4343. | 1.9 | 1 |
| 853 | Investigation of the difference in color enhancement effect on cyanidin-3-O-glucoside by phenolic acids and the interaction mechanism. Food Chemistry, 2023, 411, 135409. | 4.2 | 1 |
| 854 | Substituent effects on helical structures and chiroptical properties of fused anthracenes with bulky phenyl groups. Tetrahedron, 2023, 132, 133243. | 1.0 | 2 |
| 855 | The role of nature of aromatic ring on cooperativity between Ï€â€“Ï€ stacking and ionâ€“Ï€ interactions: A computational study. Computational and Theoretical Chemistry, 2023, 1220, 114022. | 1.1 | 2 |
| 856 | The two-pronged approach of heteroatoms and substituents to achieve a synergistic regulation of the ESIPT process in amino 2-(2â€²-hydroxyphenyl)benzoxazole derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 291, 122318. | 2.0 | 4 |
| 857 | Molecular adsorption on coinage metal subnanoclusters: A <scp>DFT</scp> + <scp>D3</scp> investigation. Journal of Computational Chemistry, 0, , . | 1.5 | 1 |
| 858 | Stability and hydrogen storage properties of Sc6O8 and Y6O8 cage-like complexes. International Journal of Hydrogen Energy, 2023, , . | 3.8 | 0 |
| 859 | A theoretical study of Mâ€“Mâ€² polar-covalent bonding in heterobimetallic multinuclear organometallic complexes of monovalent group 11 metal centres. Physical Chemistry Chemical Physics, 2023, 25, 7642-7647. | 1.3 | 1 |
| 860 | Computational study of the interaction of the psychoactive amphetamine with 1,2-indanedione and 1,8-diazafluoren-9-one as fingerprinting reagents. RSC Advances, 2023, 13, 4077-4088. | 1.7 | 0 |
| 861 | A specific MNDO parameterization for water. Journal of Chemical Physics, 2023, 158, . | 1.2 | 1 |
| 862 | Electronic structure and density functional theory. , 2023, , 3-35. | | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 863 | Molecular Dynamics with Chemical Accuracyâ”€Alkane Adsorption in Acidic Zeolites. ACS Catalysis, 2023, 13, 2011-2024. | 5.5 | 5 |
| 864 | Accuracy of Intermolecular interaction Energies, Particularly Those of Hetero Atom Containing Molecules Obtained by van der Waals DFT Calculations. ChemistrySelect, 2023, 8, . | 0.7 | 1 |
| 865 | Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections. Physical Chemistry Chemical Physics, 2023, 25, 12259-12276. | 1.3 | 4 |
| 866 | Pressure-induced second-order phase transition in fluorine. Physical Chemistry Chemical Physics, 2023, 25, 9935-9943. | 1.3 | 1 |
| 867 | Role of Hydrogen Bond Defects for Cluster Formation and Distribution in Ionic Liquids by Means of Neutron Diffraction and Molecular Dynamics Simulations. ChemPhysChem, 2023, 24, . | 1.0 | 1 |
| 868 | Ion-Neutral Collision Cross Section as a Function of the Static Dipole Polarizability and the Ionization Energy of the Ion. Journal of Physical Chemistry A, 2023, 127, 3274-3280. | 1.1 | 1 |
| 869 | Triazole based Schiff bases and their oxovanadium(IV) complexes: Synthesis, characterization, antibacterial assay, and computational assessments. Heliyon, 2023, 9, e15239. | 1.4 | 6 |
| 870 | Dependence of predicted bulk properties of hexagonal hydroxyapatite on exchangeâ€“correlation functional. Computational Materials Science, 2023, 224, 112153. | 1.4 | 5 |
| 871 | Construction of amphiphilic and polyoxometalate poly(ionic liquids) for enhanced oxidative desulfurization in fuel. Journal of Molecular Liquids, 2023, 379, 121650. | 2.3 | 5 |
| 872 | How an electric field makes endohedral fullerene an improved catalyst for hydrogen evolution reaction. Computational and Theoretical Chemistry, 2023, 1221, 114026. | 1.1 | 3 |
| 873 | Effects of dispersion corrections on the theoretical description of bulk metals. Physical Review B, 2023, 107, . | 1.1 | 5 |
| 874 | From 8- to 18-Cluster Electrons Superatoms: Evaluation via DFT Calculations of the Ligand-Protected W@Au<sub>12</sub>(dppm)<sub>6</sub> Cluster Displaying Distinctive Electronic and Optical Properties. Inorganic Chemistry, 2023, 62, 3047-3055. | 1.9 | 3 |
| 875 | Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study. ChemPhysChem, 0, , . | 1.0 | 1 |
| 876 | Generalized Many-Body Dispersion Correction through Random-Phase Approximation for Chemically Accurate Density Functional Theory. Journal of Physical Chemistry Letters, 2023, 14, 1609-1617. | 2.1 | 3 |
| 877 | Comparative First-Principles Study on Tetravalent Ion-Incorporated MTW-Type Zeolites. Journal of Physical Chemistry C, 2023, 127, 3837-3848. | 1.5 | 0 |
| 878 | Model Chemistry Recommendations for Scaled Harmonic Frequency Calculations: A Benchmark Study. Journal of Physical Chemistry A, 2023, 127, 1715-1735. | 1.1 | 19 |
| 879 | Noncovalent Interactions in Crowded Benzene Systems: How Much Strain Is Too Much? Attractions Overcome Repulsions!. Synlett, 0, , . | 1.0 | 0 |
| 880 | The Boekelheide Rearrangement of Pyrimidine Nâ€oxides as a Case Study of Closed or Open Shell Reactions â€•Experimental and Computational Evidence for the Participation of Radical Intermediates. Chemistry - A European Journal, 2023, 29, . | 1.7 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 881 | Toward Pair Atomic Density Fitting for Correlation Energies with Benchmark Accuracy. Journal of Chemical Theory and Computation, 2023, 19, 1499-1516. | 2.3 | 8 |
| 882 | Exploring alkali metal cationâ‹¯hydrogen interaction in the formation half sandwich complexes with cycloalkanes: a DFT approach. Pure and Applied Chemistry, 2023, . | 0.9 | 0 |
| 883 | Enantiopurification of Mandelic Acid by Crystallization-Induced Diastereomer Transformation: An Experimental and Computational Study. Crystal Growth and Design, 2023, 23, 2001-2010. | 1.4 | 2 |
| 884 | Machine Learning Interatomic Potentials and Long-Range Physics. Journal of Physical Chemistry A, 2023, 127, 2417-2431. | 1.1 | 19 |
| 885 | Editorial: Fragment-based electronic structure methods for solids. Frontiers in Chemistry, 0, 11, . | 1.8 | 0 |
| 886 | Mechanism and Selectivity of Copper-Catalyzed Bromination of Distal C(sp‹sup›3‹/sup›)â€“H Bonds. Organometallics, 2023, 42, 2467-2476. | 1.1 | 1 |
| 887 | Anomalous thickness dependence of photoluminescence quantum yield in black phosphorous. Nature Nanotechnology, 2023, 18, 507-513. | 15.6 | 16 |
| 888 | Functional group corrections to the GFN2-xTB and PM6 semiempirical methods for noncovalent interactions in alkanes and alkenes. Journal of Chemical Physics, 2023, 158, . | 1.2 | 1 |
| 889 | Decomposing Chemical Space: Applications to the Machine Learning of Atomic Energies. Journal of Chemical Theory and Computation, 2023, 19, 2029-2038. | 2.3 | 3 |
| 890 | Synthesis of an aqueous, air-stable, superconducting 1Tâ€²-WS ‹sub›2‹/sub› monolayer ink. Science Advances, 2023, 9, . | 4.7 | 10 |
| 891 | Understanding and Describing London Dispersion Effects in ÂTransition-Metal-Catalyzed Câ€“H Activations. Synlett, 2023, 34, 1098-1112. | 1.0 | 1 |
| 892 | CO and CO‹sub›2‹/sub› adsorption mechanism in Fe(pz)[Pt(CN)‹sub›4‹/sub›] probed by neutron scattering and density-functional theory calculations. Physical Chemistry Chemical Physics, 0, , . | 1.3 | 1 |
| 894 | Dispersion in Crystal Structures of 1-Chloro-3-aryl-5-trihalomethyl-1Î»4,2,4,6-thiatriazines: Towards an Understanding of the Supramolecular Organization of Covalent Thiazyl Chlorides. Synlett, 2023, 34, 1113-1121. | 1.0 | 3 |
| 895 | Hydrogen adsorption on lithium clusters coordinated to a gC3N4 cavity. Journal of Molecular Graphics and Modelling, 2023, 122, 108491. | 1.3 | 1 |
| 896 | L-Histidine-based computation devices. Pramana - Journal of Physics, 2023, 97, . | 0.6 | 1 |
| 897 | Investigating the Structural, Electronic, and Topological Properties of [BMIm][Fe(NO)‹sub›2‹/sub›Cl‹sub›2‹/sub›] Magnetic Ionic Liquid: Density Functional Theory Approaches. Journal of Physical Chemistry B, 2023, 127, 3787-3797. | 1.2 | 1 |
| 898 | Ab Initio Molecular Dynamics: A Guide to Applications. , 2024, , 493-517. | | 0 |
| 906 | How to make symmetry-adapted perturbation theory more accurate?. Advances in Quantum Chemistry, 2023, , 37-72. | 0.4 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 909 | Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93. | | 0 |
| 912 | Approaching Coupled Cluster Accuracy with Density Functional Theory Using the Generalized Connectivity-Based Hierarchy. Journal of Chemical Theory and Computation, 2023, 19, 3763-3778. | 2.3 | 2 |
| 913 | First-principles modeling of dye-sensitized solar cells: From the optical properties of standalone dyes to the charge separation at dye/TiO2 interfaces. , 2023, , 215-245. | | 1 |
| 915 | Density-Derived Electrostatic and Chemical Methods. , 2024, , 362-405. | | 1 |
| 923 | Application of Molecular Simulation Methods in Treating Intrinsic Structures of Energetic Materials. , 2023, , 41-113. | | 1 |
| 966 | Benchmarks for transition metal spin-state energetics: why and how to employ experimental reference data?. Physical Chemistry Chemical Physics, 2023, 25, 30800-30820. | 1.3 | 0 |
| 970 | Density Functional Theory Calculations for Materials with Complex Structures. The Materials Research Society Series, 2024, , 187-216. | 0.2 | 0 |
| 995 | The quest for superheavy elements and the limit of the periodic table. Nature Reviews Physics, 2024, 6, 86-98. | 11.9 | 1 |
| 1028 | Theoretical Understanding and Insights on Flexible Metalâ€“Organic Frameworks. , 2024, , 231-303. | | 0 |