

CITATION REPORT

List of articles citing

Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package

DOI: 10.1063/5.0055522

Journal of Chemical Physics, 2021, 155, 084801.

Source: <https://exaly.com/paper-pdf/81627092/citation-report.pdf>

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
278	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singlet-Triplet Gaps with Chemical Accuracy from Open-Shell Kohn-Sham Reaction-Field Calculations. 2021 , 12, 8470-8480		7
277	Insights on the site-selective fragmentation of CF ₂ Cl ₂ and CH ₂ Cl ₂ at the chlorine K-edge from ab initio calculations. 2021 , 548, 111226		0
276	CAP/EA-ADC method for metastable anions: Computational aspects and application to π resonances of norbornadiene and 1,4-cyclohexadiene. <i>Journal of Chemical Physics</i> , 2021 , 155, 054103	3.9	2
275	Molecular Dynamics Simulations of Bimolecular Electron Transfer: the Distance-Dependent Electronic Coupling. 2021 , 125, 10527-10537		2
274	MB-Fit: Software infrastructure for data-driven many-body potential energy functions. <i>Journal of Chemical Physics</i> , 2021 , 155, 124801	3.9	8
273	A Two-Step Baromechanical Cycle for Repeated Activation and Deactivation of Mechanophores. 2021 , 12, 9470-9474		
272	-Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. 2021 , 23, 24016-24028		0
271	QM/MM modeling of class A β -lactamases reveals distinct acylation pathways for ampicillin and cefalexin. 2021 , 19, 9182-9189		1
270	Challenges for variational reduced-density-matrix theory with three-particle N-representability conditions. <i>Journal of Chemical Physics</i> , 2021 , 155, 174110	3.9	2
269	Molecular Magnetizabilities Computed Via Finite Fields: Assessing Alternatives to MP2 and Revisiting Magnetic Exaltations in Aromatic and Antiaromatic Species.. 2021 , 119,		
268	Computational Investigation of the Formation of Substituted Isoindole -Oxides through the Photo-oxidative Cyclization of 2'-Alkynylacetophenone Oximes. 2021 , 86, 15020-15032		
267	Stereodynamic Control of Collision-Induced Nonadiabatic Dynamics of NO (π) with H, N, and CO: Intermolecular Interactions Drive Collision Outcomes. 2021 , 125, 8803-8815		1
266	Approaching the basis set limit in Gaussian-orbital-based periodic calculations with transferability: Performance of pure density functionals for simple semiconductors. <i>Journal of Chemical Physics</i> , 2021 , 155, 164102	3.9	4
265	Crossed Beam Experiments and Computational Studies of Pathways to the Preparation of Singlet Ethynylsilylene (HCCSiH; XA'): The Silacarbene Counterpart of Triplet Propargylene (HCCCH; XB). 2021 , 12, 10768-10776		2
264	Direct Dynamics with Nuclear-Electronic Orbital Density Functional Theory. 2021 , 54, 4131-4141		7
263	Interaction Energy Analysis of Monovalent Inorganic Anions in Bulk Water Versus Air/Water Interface. 2021 , 26,		2
262	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. 2021 , 12, 6359		9

261	The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in push-pull chromophores. 2021 , 23, 26135-26150		2
260	Buffer concentration dramatically affects the stability of S-nitrosothiols in aqueous solutions. 2021 , 118, 59-65		0
259	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Bicyclic Systems. 2021 , 125, 10174-10188		0
258	OpenMechanochem: A Python module for mechanochemical simulations. 2021 , 16, 100879		
257	Photoredox Chemistry with Organic Catalysts: Role of Computational Methods.. 2021 , 6, 33253-33264		0
256	Dissociation of HCl in water nanoclusters: an energy decomposition analysis perspective. 2021 , 23, 26737-26749		
255	Vibronic Coupling Effect on the Vibrationally Resolved Electronic Spectra and Intersystem Crossing Rates of a TADF Emitter: 7-PhQAD.. 2022 ,		6
254	libwfa: Wavefunction analysis tools for excited and open-shell electronic states.		2
253	MacroQC 1.0: An electronic structure theory software for large-scale applications.. <i>Journal of Chemical Physics</i> , 2022 , 156, 044801	3.9	1
252	Influence of N-introduction in pentacene on the electronic structure and excited electronic states.. 2022 ,		0
251	Simple evaluation of dynamic disorder effects on exciton transport.. <i>Journal of Chemical Physics</i> , 2022 , 156, 044112	3.9	
250	Quantifying Fluctuations of Average Solvent Environments for Embedding Calculations.. 2022 ,		1
249	OS100: A Benchmark Set of 100 Digitized UV-Visible Spectra and Derived Experimental Oscillator Strengths.. 2022 ,		1
248	Path-dependency of energy decomposition analysis & the elusive nature of bonding.. 2022 ,		4
247	A computational study of the mechanism of chloroalkane dechlorination with Rh(I) complexes.. 2022 ,		0
246	Ultrasensitive and multiplex SERS determination of anthropogenic phenols in oil fuel and environmental samples.		1
245	Interplay Between Applied Force and Radical Attack in the Mechanochemical Chain Scission of Poly(acrylic acid).. 2022 ,		
244	Cyclopentannulated Dihydropentazapentacenes.. 2022 ,		0

243	Excited state absorption of DNA bases in the gas phase and in chloroform solution: a comparative quantum mechanical study.. 2022 ,		1
242	Ultrafast Dynamics of Nitro-Nitrite Rearrangement and Dissociation in Nitromethane Cation.. 2022 ,		1
241	Vertical ionization potential benchmark for unitary coupled-cluster and algebraic-diagrammatic construction methods.. <i>Journal of Chemical Physics</i> , 2022 , 156, 054114	3.9	2
240	Regularized Second-Order Møller-Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost.. 2021 , 12, 12084-12097		6
239	Intramolecular hydrogen transfer in DNA induced by site-selective resonant core excitation.. 2022 ,		0
238	Transition Structures, Reaction Paths, and Kinetics: Methods and Applications in Catalysis. 2022 ,		
237	Generation of multiple triplet states in an orthogonal bodipy dimer: a breakthrough spectroscopic and theoretical approach.. 2022 ,		1
236	Kinetics and mechanistic details of bulk ZnO dissolution using a thiol-imidazole system.. 2022 , 13, 3208-3215		0
235	Energy Landscape of State-Specific Electronic Structure Theory.. 2022 ,		3
234	Investigation of Thermally Activated Delayed Fluorescence in Donor-Acceptor Organic Emitters with Time-Resolved Absorption Spectroscopy. 2022 , 34, 2161-2175		1
233	LMoDeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis.. 2022 , 18, 1821-1837		0
232	Probing Molecular Chirality of Ground and Electronically Excited States in the UV-vis and X-ray Regimes: An EOM-CCSD Study.. 2022 ,		2
231	The many-body electronic interactions of Fe(II)-porphyrin.. <i>Journal of Chemical Physics</i> , 2022 , 156, 094110	3.9	1
230	Cavity quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. II. Analytic energy gradient.. <i>Journal of Chemical Physics</i> , 2022 , 156, 124104	3.9	1
229	Exploring the accuracy and usefulness of semi-empirically scaled ADC schemes by blending second and third order terms.. <i>Journal of Chemical Physics</i> , 2022 , 156, 144101	3.9	1
228	Optimizing the Solvent Reorganization Free Energy by Metal Substitution for Nanocage Catalysis. 2022 , 12, 3782-3788		2
227	Appraisal of dispersion damping functions for the effective fragment potential method.		
226	Projected CAP-EOM-CCSD method for electronic resonances.. <i>Journal of Chemical Physics</i> , 2022 , 156, 094108	3.9	1

225	Unbiasing fermionic quantum Monte Carlo with a quantum computer.. 2022 , 603, 416-420		10
224	Comprehensive Basis-Set Testing of Extended Symmetry-Adapted Perturbation Theory and Assessment of Mixed-Basis Combinations to Reduce Cost.. 2022 ,		3
223	Molecular Auger decay rates from complex-variable coupled-cluster theory.. <i>Journal of Chemical Physics</i> , 2022 , 156, 114117	3.9	1
222	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)-Cyclobutadiene Complex.		
221	Revisiting the Bonding Model for Gold(I) Species: The Importance of Pauli Repulsion Revealed in a Gold(I)-Cyclobutadiene Complex.. 2022 ,		3
220	Pillar[4]arene[1]thioarene: Synthesis and Host-Guest Binding Properties.		
219	A Computational and Experimental View of Hydrogen Bonding in Glycerol Water Clusters.. 2022 ,		1
218	Analytical gradients for nuclear-electronic orbital multistate density functional theory: Geometry optimizations and reaction paths.. <i>Journal of Chemical Physics</i> , 2022 , 156, 114115	3.9	0
217	Transferability of data-driven, many-body models for CO simulations in the vapor and liquid phases.. <i>Journal of Chemical Physics</i> , 2022 , 156, 104503	3.9	3
216	Modeling and Characterization of Exciplexes in Photoredox CO Reduction: Insights from Quantum Chemistry and Fluorescence Spectroscopy.. 2022 ,		1
215	Coherent Control of Molecular Dissociation by Selective Excitation of Nuclear Wave Packets.. 2022 , 10, 859095		2
214	Improving Results by Improving Densities: Density-Corrected Density Functional Theory.. 2022 ,		7
213	Rational Synthesis of Ruthenium-Based Metallo-Supramolecular Polymers as Heterogeneous Catalysts for Catalytic Transfer Hydrogenation of Carbonyl Compounds. 2022 , 121383		0
212	Dewar benzenoids in cyclophenacene nanobelts. 2022 , 797, 139576		0
211	Interactions of N-hydroxyamphetamine with an iron porphyrin: A unique intramolecular H-bond probed by DFT calculations.. 2022 , 231, 111779		
210	Accelerating the Convergence of Self-Consistent Field Calculations Using the Many-Body Expansion. 2021 ,		1
209	Oxidation State Localized Orbitals: A Method for Assigning Oxidation States Using Optimally Fragment-Localized Orbitals and a Fragment Orbital Localization Index.. 2021 ,		1
208	Linear Combination of Atomic Dipoles to Calculate the Bond and Molecular Dipole Moments of Molecules and Molecular Liquids.. 2021 , 12, 12360-12369		1

207	Erratum: "Harnessing the meta-generalized gradient approximation for time-dependent density functional theory" [J. Chem. Phys. 137, 164105 (2012)].. <i>Journal of Chemical Physics</i> , 2022 , 156, 159902	3.9	3
206	Reformulation of thermally assisted-occupation density functional theory in the Kohn-Sham framework.. <i>Journal of Chemical Physics</i> , 2022 , 156, 174108	3.9	0
205	Relativistic Orbital-Optimized Density Functional Theory for Accurate Core-Level Spectroscopy.. 2022 , 3438-3449		5
204	Computationally Probing the Mechanism of the Blue-Light-Driven O-H Functionalization of Alcohols by Aryldiazoacetates: Photobasicity or Carbene Chemistry.. 2022 ,		1
203	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark.. 2022 , 3499-3506		3
202	Semiclassical Real-Time Nuclear-Electronic Orbital Dynamics for Molecular Polaritons: Unified Theory of Electronic and Vibrational Strong Couplings.. 2022 ,		3
201	Deciphering Distinct Overpotential-Dependent Pathways for Electrochemical CO Reduction Catalyzed by an Iron-Terpyridine Complex.. 2022 ,		0
200	Rationalization and tuning of doublet emission in organic radicals.		
199	Using core-hole reference states for calculating X-ray photoelectron and emission spectra.. 2022 ,		3
198	Providing theoretical insight into the role of symmetry in the photoisomerization mechanism of a non-symmetric dithienylethene photoswitch.. 2022 ,		0
197	Predicting Reaction Conditions from Limited Data through Active Transfer Learning.		1
196	A matrix completion algorithm for efficient calculation of quantum and variational effects in chemical reactions.. <i>Journal of Chemical Physics</i> , 2022 , 156, 184119	3.9	1
195	Complex Energies and Transition-Dipoles for the Uracil anion Shape-type Resonances from stabilization curves via Pad� <i>Journal of Chemical Physics</i> ,	3.9	0
194	State-specific solvation for restricted active space spin-flip (RAS-SF) wave functions based on the polarizable continuum formalism. <i>Journal of Chemical Physics</i> ,	3.9	
193	Comparison of approximate intermolecular potentials for ab initio fragment calculations on medium sized N-heterocycles.. 2022 ,		1
192	Organic photoredox catalysts for CO reduction: Driving discovery with genetic algorithms.. <i>Journal of Chemical Physics</i> , 2022 , 156, 184109	3.9	3
191	Expansion of 2,3,6,7-Tetraazanaphthalene with Two Embedded Heptagons: Highly Twisted Structure and Lone-Pair/� Interaction in the Crystal.. 2022 ,		1
190	Nuclear-Electronic Orbital Approach to Quantization of Protons in Periodic Electronic Structure Calculations. <i>Journal of Chemical Physics</i> ,	3.9	

189	Revisiting the Performance of Time-Dependent Density Functional Theory for Electronic Excitations: Assessment of 43 Popular and Recently Developed Functionals from Rungs One to Four.. 2022 ,		4
188	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water.. 2022 ,		2
187	A two-directional vibrational probe reveals different electric field orientations in solution and an enzyme active site.. 2022 ,		2
186	Computing X-Ray Absorption Spectra from Linear-Response Particles atop Optimized Holes. <i>Journal of Chemical Physics</i> ,	3.9	2
185	Core-hole delocalization for modeling X-ray spectroscopies: A cautionary tale. <i>Journal of Chemical Physics</i> ,	3.9	1
184	High harmonic spectra computed using time-dependent Kohn-Sham theory with Gaussian orbitals and a complex absorbing potential. <i>Journal of Chemical Physics</i> ,	3.9	1
183	Efficient implementation of molecular CCSD gradients with Cholesky-decomposed electron repulsion integrals. <i>Journal of Chemical Physics</i> ,	3.9	0
182	A benchmark dataset for Hydrogen Combustion.. 2022 , 9, 215		0
181	Evaluation of Molecular Photophysical and Photochemical Properties Using Linear Response Time-Dependent Density Functional Theory with Classical Embedding: Successes and Challenges. <i>Journal of Chemical Physics</i> ,	3.9	1
180	Conformational Energy Benchmark for Longer n-Alkane Chains.		2
179	Assessing the stability of Pd-exchanged sites in zeolites with the aid of a high throughput quantum chemistry workflow. 2022 , 13,		2
178	Obtaining QM/MM binding free energies in the SAMPL8 drugs of abuse challenge: indirect approaches.		1
177	Computational investigation of substituent effects on the fluorescence wavelengths of oxyluciferin analogs. 2022 , 431, 114018		
176	Methods to Calculate Electronic Excited-State Dynamics for Molecules on Large Metal Clusters with Many States: Ensuring Fast Overlap Calculations and a Robust Choice of Phase.		1
175	Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways.		0
174	Role of Dielectric Screening in Calculating Excited States of Solvated Azobenzene: A Benchmark Study Comparing Quantum Embedding and Polarizable Continuum Model for Representing the Solvent. 4849-4855		1
173	Pushing steric limits in osmium(IV) tetraaryl complexes.		
172	Photochemically triggered cheletropic formation of cyclopropenone (c-C ₃ H ₂ O) from carbon monoxide and electronically excited acetylene.		0

171	Toward Efficient Direct Dynamics Studies of Chemical Reactions: A Novel Matrix Completion Algorithm.		1
170	Gas-Phase Peroxyl Radical Recombination Reactions: A Computational Study of Formation and Decomposition of Tetroxides.		1
169	Analytic Gradients for the Long-Range-Corrected XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Assessment. 2022 , 126, 3937-3946		
168	How Reliable Are Modern Density Functional Approximations to Simulate Vibrational Spectroscopies?. 5963-5968		1
167	Eliminating the Reverse ISC Bottleneck of TADF Through Excited State Engineering and Environment-Tuning Toward State Resonance Leading to Mono-Exponential Sub- μ s Decay. High OLED External Quantum Efficiency Confirms Efficient Exciton Harvesting. 2201772		0
166	Graph-Learning Guided Mechanistic Insights into Imipenem Hydrolysis in GES Carbapenemases.		0
165	Multicomponent Orbital-Optimized Perturbation Theory with Density Fitting: Anharmonic Zero-Point Energies in Protonated Water Clusters. 2022 , 13, 5563-5570		0
164	Detection and Correction of Delocalization Errors for Electron and Hole Polarons Using Density-Corrected DFT. 5275-5284		0
163	Spin-density calculation via the graphical unitary group approach.		1
162	Near-Exact Nuclear Gradients of Complete Active Space Self-Consistent Field Wave Functions. <i>Journal of Chemical Physics</i> ,	3.9	0
161	Magnetic exchange interactions in binuclear and tetranuclear iron(III) complexes described by spin-flip DFT and Heisenberg effective Hamiltonians.		3
160	Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. <i>Journal of Chemical Physics</i> ,	3.9	1
159	Introduction to special issue: Chaos Indicators, Phase Space and Chemical Reaction Dynamics. 2022 , 439, 133385		0
158	Electronic structure of substituted catecholate complexes of hexacoordinated silicon: a quantum chemical study. 2022 , 71, 1111-1122		
157	Coupled Cluster Benchmarking of Large Noncovalent Complexes in L7 and S12L as Well as the C60 Dimer, DNA Ellipticine, and HIV Inhibitor. 2022 , 126, 4326-4341		4
156	Initiator enhancement of mandrel degradation for ICF target fabrication. 2022 , 104733		
155	How Reproducible Are QM/MM Simulations? Lessons from Computational Studies of the Covalent Inhibition of the SARS-CoV-2 Main Protease by Carmofur.		2
154	Exchange Coupling Determines Metal-Dependent Efficiency for Iron- and Cobalt-Catalyzed Photochemical CO ₂ Reduction. 2022 , 12, 8484-8493		0

153	N-representability of the target density in Frozen-Density Embedding Theory based methods: numerical significance and its relation to electronic polarisation. <i>Journal of Chemical Physics</i> ,	3.9	0
152	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the HartreeFock Density?.		2
151	Reference Energies for Cyclobutadiene: Automerization and Excited States.		2
150	Accelerated Multiphosphorylated Peptide Synthesis.		1
149	Non-iterative Method for Constructing Valence Antibonding Molecular Orbitals and a Molecule-adapted Minimum Basis.. <i>Journal of Chemical Physics</i> ,	3.9	2
148	Quantifying and reducing spin contamination in algebraic diagrammatic construction theory of charged excitations. <i>Journal of Chemical Physics</i> ,	3.9	
147	Proton-coupled energy transfer in molecular triads.		0
146	INAQS, a Generic Interface for Nonadiabatic QM/MM Dynamics: Design, Implementation, and Validation for GROMACS/Q-CHEM simulations. 2022 , 18, 4601-4614		1
145	Observation of intermolecular Coulombic decay and shake-up satellites in liquid ammonia. 2022 , 9, 044901		0
144	Targeting the Major Groove of the Palindromic d(GGCGCC) ₂ Sequence by Oligopeptide Derivatives of Anthraquinone Intercalators.		1
143	Application of Box and Voronoi CAPs for Metastable Electronic States in Molecular Clusters. 2022 , 126, 5070-5078		
142	Solvent Organization and Electrostatics Tuned by Solute Electronic Structure: Amide versus Non-Amide Carbonyls. 2022 , 126, 5876-5886		
141	Trade-Off between Redox Potential and the Strength of Electrochemical CO ₂ Capture in Quinones. 2022 , 126, 14163-14172		0
140	Can a Finite Chain of Hydrogen Cyanide Molecules Model a Crystal?.		1
139	Channel-specific core-valence projectors for determining partial Auger decay widths.		0
138	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. 2022 , 126, 5492-5505		1
137	Solvent Dependent Nuclear Magnetic Resonance Molecular Parameters Based on a Polarization Consistent Screened Range Separated Hybrid Density Functional Theory Framework.		
136	On the prospects of optical cycling in diatomic cations: effects of transition metals, spin-orbit couplings, and multiple bonds.		

- 135 Designing boron-cluster-centered zwitterionic Y-shaped clocked QCA molecules. 1
- 134 Visualization of electron density changes along chemical reaction pathways.
- 133 Changes in polarization dictate necessary approximations for modeling electronic deexcitation intensity: Application to x-ray emission. **2022**, 106, 0
- 132 A-value revisited: ring flip energy of chair structures in halogenated cyclohexanes by quantum chemical methods. 0
- 131 Optoelectronic properties of a self-assembling rigidly-linked BF₂-curcuminoid bichromophore. **2022**, 207, 110677 0
- 130 TTDFT: A GPU accelerated Tucker tensor DFT code for large-scale Kohn-Sham DFT calculations. **2023**, 282, 108516 0
- 129 A computational mechanistic study of CH hydroxylation with mononuclear copper-oxygen complexes. 0
- 128 Accurate core excitation and ionization energies from a state-specific coupled-cluster singles and doubles approach. **2022**, 24, 20728-20741 2
- 127 A self-crosslinking monomer, β -pinene methacrylate: understanding and exploiting hydrogen abstraction. 1
- 126 The role of the intermediate triplet state in iron-catalyzed multi-state C-H activation. **2022**, 24, 20721-20727 1
- 125 The impact of G-quadruplex dynamics on inter-tetrad electronic couplings: a hybrid computational study. **2022**, 24, 22513-22522 0
- 124 Jahn-Teller distortion and dissociation of CCl₄⁺ by transient X-ray spectroscopy simultaneously at the carbon K- and chlorine L-edge. **2022**, 13, 9310-9320 3
- 123 Side-chain engineering for high degradation performance of mandrel materials in ICF target fabrication. 0
- 122 Data-Driven Many-Body Potential Energy Functions for Generic Molecules: Linear Alkanes as a Proof-of-Concept Application. 1
- 121 Ab Initio Molecular Dynamics of Temporary Anions Using Complex Absorbing Potentials. **2022**, 13, 8477-8483 1
- 120 Synergistic interplay between photoisomerization and photoluminescence in a light-driven rotary molecular motor. **2022**, 13, 0
- 119 Static Electron Correlation in Anharmonic Molecular Vibrations: A Hybrid TAO-DFT Study. 1
- 118 Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. 2

117	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.	10
116	Revisiting the Orbital Energy-Dependent Regularization of Orbital-Optimized Second-Order Møller-Plesset Theory. 2022 , 18, 5382-5392	1
115	Frozen-Density Embedding for Including Environmental Effects in the Dirac-Kohn-Sham Theory: An Implementation Based on Density Fitting and Prototyping Techniques.	0
114	Synthesis, Crystal Structure, and Properties of Phenylsilicon(IV) Bis-catecholate Complexes. 2022 , 48, 647-658	0
113	Extended Ligands in Two-Coordinate Coinage Metal Complexes. 2022 , 144, 17916-17928	0
112	Cherry-Picking Resolvents: Recovering the Valence Contribution in X-ray Two-Photon Absorption within the Core-Valence-Separated Equation-of-Motion Coupled-Cluster Response Theory.	1
111	ClearRIXS: A fast and accurate first-principles method for simulation and analysis of resonant inelastic x-ray scattering. 2022 , 106,	0
110	Analytic High-Order Energy Derivatives for Metal Nanoparticle-Mediated Infrared and Raman Scattering Spectra within the Framework of Quantum Mechanics/Molecular Mechanics Model with Induced Charges and Dipoles.	0
109	M-Chem: a modular software package for molecular simulation that spans scientific domains.	0
108	Ultrafast Evaluation of Two-Photon Absorption with Simplified Time-Dependent Density Functional Theory.	0
107	Magnetic circular dichroism within the Algebraic Diagrammatic Construction scheme of the polarisation propagator up to third order.	1
106	Controlling the fluorescence quantum yields of benzothiazole-difluoroborates by optimal substitution.	0
105	S66x8 noncovalent interactions revisited: new benchmark and performance of composite localized coupled-cluster methods. 2022 , 24, 25555-25570	1
104	Reactive quenching of NO (A ² Σ) with H ₂ O leads to HONO: a theoretical analysis of the reactive and nonreactive electronic quenching mechanisms.	0
103	A spin- $\frac{1}{2}$ variant of the second-order approximate coupled-cluster singles and doubles method.	0
102	On the choice of reference orbitals for linear-response calculations of solution-phase K-edge X-ray absorption spectra. 2022 , 24, 26170-26179	0
101	Research on task scheduling scheme for quantum computing cloud platform. 2022 ,	0
100	Computational Study on the Effect of Thienyl Donor on the Optical Response of Nonclassical Oligo-Pyrazinothienothiadiazole Biradicaloids. 2022 , 126, 7829-7839	0

99	Systematic Evaluation of Counterpoise Correction in Density Functional Theory.	3
98	Accurate Prediction of Vertical Ionization Potentials and Electron Affinities from Spin-Component Scaled CC2 and ADC(2) Models.	0
97	Reorganization Energies for Interfacial Proton-Coupled Electron Transfer to a Water Oxidation Catalyst.	0
96	Sella, an Open-Source Automation-Friendly Molecular Saddle Point Optimizer.	0
95	The fourth-order algebraic diagrammatic construction scheme for the polarization propagator.	1
94	Correcting delocalisation errors in conformational energies using density-corrected DFT, with application to crystal polymorphs.	0
93	Comparative Analysis of Uncoupled Mode Approximations for Molecular Thermochemistry and Kinetics.	1
92	Recent Advances toward Efficient Calculation of Higher Nuclear Derivatives in Quantum Chemistry. 2022 , 126, 7795-7805	1
91	Many recent density functionals are numerically ill-behaved.	1
90	Twenty Years of Auxiliary-Field Quantum Monte Carlo in Quantum Chemistry: An Overview and Assessment on Main Group Chemistry and Bond-Breaking.	1
89	Nano-crystalline precursor formation, stability, and transformation to mullite-type visible-light photocatalysts.	2
88	An efficient implementation of the GOSTSHYP pressure model by applying shell-bounding gaussian 1-electron-3-center integral screening.	0
87	Electron-Affinity Time-Dependent Density Functional Theory: Formalism and Applications to Core-Excited States. 2022 , 13, 9664-9672	1
86	High Resolution Photoelectron Spectroscopy of the Acetyl Anion. 2022 , 126, 7962-7970	1
85	Prediction of Multiple Hydrogen Ligation at a Vanadium(II) Site in a Metal-Organic Framework. 10471-10478	2
84	Disentangling the Resonant Auger Spectra of Ozone: Overlapping Core-Hole States and Core-Excited State Dynamics.	1
83	Core spectroscopy of oxazole.	0
82	FCclasses3 : Vibrationally-resolved spectra simulated at the edge of the harmonic approximation.	1

81	Nonadiabatic Dynamics of Hydrogen Tunneling with Nuclear-Electronic Orbital Multistate Density Functional Theory.	2
80	Spectroscopic signatures of states in the continuum characterized by a joint experimental and theoretical study of pyrrole.	2
79	Conceptual Density Functional Theory for Temporary Anions Stabilized by Scaled Nuclear Charges.	0
78	Generalization of ETS-NOCV and ALMO-COVP Energy Decomposition Analysis to Connect Any Two Electronic States and Comparative Assessment.	2
77	Predictive stochastic analysis of massive filter-based electrochemical reaction networks.	0
76	DFT calculations in solution systems: solvation energy, dispersion energy and entropy.	0
75	Multivalent optical cycling centers: towards control of polyatomics with multi-electron degrees of freedom. 2022 , 25, 154-170	0
74	Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning.	0
73	A comprehensive benchmark investigation of quantum chemical methods for carbocations.	0
72	Does GLPT2 offer any actual benefit over conventional HF-MP2 in the context of double-hybrid density functionals?. 2022 ,	1
71	Reliable prediction of association (free) energies of supramolecular complexes with heavy main group elements in the HS13L benchmark set. 2022 , 24, 28831-28843	0
70	Analytical gradients and derivative couplings for the TDDFT-1D method.	0
69	Trapping the Transition State in a [2,3]-Sigmatropic Rearrangement by Applying Pressure. 2022 , 7, 45208-45214	
68	Either Accurate Singlet-Triplet Gaps or Excited-State Structures: Testing and Understanding the Performance of TD-DFT for TADF Emitters. 2022 , 18, 7702-7713	0
67	Charge-transfer-to-solvent states provide a sensitive spectroscopic probe of the local solvent structure around anions.	0
66	Differentiable quantum chemistry with PySCF for molecules and materials at the mean-field level and beyond. 2022 , 157, 204801	2
65	Efficient Computation of the Interaction Energies of Very Large Non-covalently Bound Complexes.	0
64	Simulations of electric field gradient fluctuations and dynamics around sodium ions in ionic liquids. 2022 , 157, 244502	0

- 63 Soft-x-ray spectroscopy of coronene+ and (coronene+H)+ cations: The influence of hydrogenation on electronic structure and ph. **2022**, 106, 0
- 62 Transition1x - a dataset for building generalizable reactive machine learning potentials. **2022**, 9, 0
- 61 Excitation and fragmentation of the dielectric gas C4F7N: electrons vs. photons. 0
- 60 Spin-orbit couplings within spin-conserving and spin-flipping time-dependent density functional theory: Implementation and benchmark calculations. **2022**, 157, 224110 2
- 59 ipie: A Python-Based Auxiliary-Field Quantum Monte Carlo Program with Flexibility and Efficiency on CPUs and GPUs. 0
- 58 Performance of Localized-Orbital Coupled-Cluster Approaches for the Conformational Energies of Longer n-Alkane Chains. **2022**, 126, 9375-9391 0
- 57 Impact of Connectivity on the Electronic Structure of N-Heterotriangulenes. 0
- 56 Building on the Strengths of a Double-Hybrid Density Functional for Excitation Energies and Inverted Singlet-Triplet Energy Gaps. 0
- 55 Perspective: Simultaneous treatment of relativity, correlation, and QED. 0
- 54 The symmetric quasi-classical model using on-the-fly time-dependent density functional theory within the Tamm-Dancoff approximation. 0
- 53 Faster Exact Exchange for Solids via occ-RI-K: Application to Combinatorially Optimized Range-Separated Hybrid Functionals for Simple Solids with Pseudopotentials Near the Basis Set Limit. **2022**, 18, 7336-7349 0
- 52 Quantum Chemical Prediction of the Acidities of Sulfonamide Inhibitors of Carbonic Anhydrase. **2022**, 126, 9207-9217 0
- 51 Efficient Calculation of NMR Shielding Constants Using Composite Method Approximations and Locally Dense Basis Sets. 0
- 50 Analytical Derivative Couplings within the Framework of Time-Dependent Density Functional Theory Coupled with Conductor-like Polarizable Continuum Model: Formalism, Implementation and Applications. 0
- 49 Theory, implementation, and disappointing results for two-photon absorption cross sections within the doubly electron-attached equation-of-motion coupled-cluster framework. 0
- 48 Ultrafast X-ray Spectroscopy of Intersystem Crossing in Hexafluoroacetylacetone: Chromophore Photophysics and Spectral Changes in the Face of Electron-Withdrawing Groups. 1
- 47 The Auger spectrum of benzene. 0
- 46 Projection-Based Density Matrix Renormalization Group in Density Functional Theory Embedding. 716-722 0

- 45 Generating accurate density matrices on the tangent space of a Grassmann manifold. ○
- 44 Improving Lurasidone Hydrochloride's Solubility and Stability by Higher-Order Complex Formation with Hydroxypropyl-β-Cyclodextrin. **2023**, 15, 232 ○
- 43 Green Electrospinning of Biodegradable Cellulose Acetate Nanofibrous Membranes with Tunable Porosity. ○
- 42 Avoiding Negligible Shell Pairs and Quartets in Electronic Structure Calculations. ○
- 41 Data-driven many-body potentials from density functional theory for aqueous phase chemistry. **2023**, 4, 011301 ○
- 40 QM/MM Modeling of Vibrational Polariton Induced Energy Transfer and Chemical Dynamics. **2023**, 145, 377-384 1
- 39 Second-Order Self-Consistent Field Algorithms: From Classical to Quantum Nuclei. ○
- 38 Mind the GAP: Quantifying the Breakdown of the Linear Vibronic Coupling Hamiltonian. ○
- 37 Spin-Orbit Couplings of Open-Shell Systems with Restricted Active Space Configuration Interaction. **2023**, 127, 1206-1218 ○
- 36 Origins of Offset-Stacking in Porous Frameworks. **2023**, 127, 2675-2686 ○
- 35 Mechanisms and Energetics for Hydrogen Abstraction of Thymine Photosensitized by Benzophenone from Theoretical Principle. ○
- 34 Symmetric Post-Transition State Bifurcation Reactions with Berry Pseudomagnetic Fields. **2023**, 14, 770-778 ○
- 33 Birth of the Hydrated Electron via Charge-Transfer-to-Solvent Excitation of Aqueous Iodide. **2023**, 14, 870-878 ○
- 32 Machine learning based implicit solvent model for aqueous-solution alanine dipeptide molecular dynamics simulations. **2023**, 13, 4565-4577 1
- 31 Electronic structure of rhombus-shaped nanographenes: system size evolution from closed- to open-shell ground states. ○
- 30 Electronic structure theory on modeling short-range noncovalent interactions between amino acids. **2023**, 158, 094301 ○
- 29 Energy Component Analysis for Electronically Excited States of Molecules: Why the Lowest Excited State Is Not Always the HOMO/LUMO Transition. ○
- 28 Electronic transition dipole moments from time-independent excited-state density-functional tight-binding. **2023**, 158, 134104 ○

- 27 An efficient implementation of analytical nuclear gradients for linear-response time-dependent density functional theory in the plane wave basis. **2023**, 5, 024003 ○
- 26 Computational insights into the antioxidant and antidiabetic mechanisms of cannabidiol: An in vitro and in silico study. **2023**, 16, 104842 ○
- 25 HOAX: a hyperparameter optimisation algorithm explorer for neural networks. ○
- 24 Ultrafast Ring Closure Reaction of Gaseous cis-Stilbene from S1(π). **2023**, 145, 3283-3288 1
- 23 Force Decomposition Analysis: A Method to Decompose Intermolecular Forces into Physically Relevant Component Contributions. **2023**, 127, 1760-1774 ○
- 22 Origin of Magnetic Anisotropy in Nickelocene Molecular Magnet and Resilience of Its Magnetic Behavior. **2023**, 127, 3647-3659 ○
- 21 New Implementation of an Equation-of-Motion Coupled-Cluster Damped-Response Framework with Illustrative Applications to Resonant Inelastic X-ray Scattering. **2023**, 127, 1775-1793 ○
- 20 Slater transition methods for core-level electron binding energies. **2023**, 158, 094111 ○
- 19 Jahn-Teller effects in initial and final states: high-resolution X-ray absorption, photoelectron and Auger spectroscopy of allene. **2023**, 25, 6733-6745 ○
- 18 Bowl-shaped carbon skeletons under tensile stress: quantum mechanochemistry of corannulene. **2023**, 47, 6050-6053 ○
- 17 Influence of Transition Metal Electron Configuration on the Structure of Metal-EDTA Complexes. **2023**, 127, 2258-2264 ○
- 16 Caught in the act: real-time observation of the solvent response that promotes excited-state proton transfer in pyranine. **2023**, 14, 4048-4058 ○
- 15 Electronic Born-Oppenheimer approximation in nuclear-electronic orbital dynamics. **2023**, 158, 114118 ○
- 14 Solvent Induced Proton Polarization within the Nuclear-Electronic Orbital Framework. **2023**, 14, 2990-2995 ○
- 13 Simple, accurate, adjustable-parameter-free prediction of NMR shifts for molecules in solution. **2023**, 25, 9952-9957 ○
- 12 Computational Studies of Rubber Ozonation Explain the Effectiveness of 6PPD as an Antidegradant and the Mechanism of Its Quinone Formation. **2023**, 57, 5216-5230 ○
- 11 Structural Sampling and Solvation Models for the Simulation of Electronic Spectra: Pyrazine as a Case Study. ○
- 10 Variable Amine Spacing Determines Depolymerization Rate in Polydiketoenamines. **2023**, 145, 8082-8089 ○

- 9 A First-Principles Investigation of Structure-Luminescence Activity of Donor-Acceptor-Donor Organic Triad. **2023**, 127, 3330-3338 ○
- 8 Exploring Bethe-Salpeter Excited-State Dipoles: The Challenging Case of Increasingly Long Push-Pull Oligomers. **2023**, 14, 3727-3734 ○
- 7 Fragment-Based Calculations of Enzymatic Thermochemistry Require Dielectric Boundary Conditions. 3826-3834 ○
- 6 Cooperative Supramolecular Polymerization of Triphenylamine bis-Urea Macrocycles. ○
- 5 A double-hybrid density functional based on good local physics with outstanding performance on the GMTKN55 database. **2023**, 158, 151103 ○
- 4 Optimized attenuated interaction: Enabling stochastic Bethe-Salpeter spectra for large systems. **2023**, 158, 154104 ○
- 3 Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. **2023**, 28, 3487 ○
- 2 Genetic drift and genome reduction in the plant pathogen *Candidatus Liberibacter solanacearum* shapes a new enzyme in lysine biosynthesis. ○
- 1 Probing Superatomic Orbitals of Sc-Doped and Undoped Silver Cluster Anions via Photoelectron Angular Anisotropy. 4011-4018 ○