Anna I Krylov

List of Publications by Year in Descending Order

259 papers	18,506 citations	67 h-index	129 g-index
278 ext. papers	20,446 ext. citations	5.6 avg, IF	7.23 L-index

#	Paper	IF	Citations
259	Royal Society of Chemistry Provides Guidelines for Censorship to its Editors. *Chemistry International*, **2022**, 44, 32-34	1.6	1
258	Scientists must resist cancel culture. *Nachrichten Aus Der Chemie*, **2022**, 70, 12-14	0.1	0
257	Role of the Electron-Dipole Interaction in Photodetachment Angular Distributions. *Journal of Physical Chemistry Letters*, **2021**, 12, 10086-10092	6.4	2
256	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2021**, 154, 114115	3.9	9
255	An assessment of different electronic structure approaches for modeling time-resolved x-ray absorption spectroscopy. *Structural Dynamics*, **2021**, 8, 024101	3.2	6
254	Is Solid Copper Oxalate a Spin Chain or a Mixture of Entangled Spin Pairs?. *Journal of Physical Chemistry C*, **2021**, 125, 7502-7510	3.8	4
253	The orbital picture of the first dipole hyperpolarizability from many-body response theory. *Journal of Chemical Physics*, **2021**, 154, 184109	3.9	1
252	Equation-of-Motion Coupled-Cluster Protocol for Calculating Magnetic Properties: Theory and Applications to Single-Molecule Magnets. *Journal of Chemical Theory and Computation*, **2021**, 17, 4225-4241	6.4	4
251	The Peril of Politicizing Science. *Journal of Physical Chemistry Letters*, **2021**, 12, 5371-5376	6.4	3
250	Photoelectron photofragment coincidence spectroscopy of aromatic carboxylates: benzoate and p-coumarate. *Physical Chemistry Chemical Physics*, **2021**, 23, 18414-18424	3.6	3
249	Interplay between Locally Excited and Charge Transfer States Governs the Photoswitching Mechanism in the Fluorescent Protein Dreiklang. *Journal of Physical Chemistry B*, **2021**, 125, 757-770	3.4	5
248	Feshbach-Fano approach for calculation of Auger decay rates using equation-of-motion coupled-cluster wave functions. I. Theory and implementation. *Journal of Chemical Physics*, **2021**, 154, 084124	3.9	5
247	Feshbach-Fano approach for calculation of Auger decay rates using equation-of-motion coupled-cluster wave functions. II. Numerical examples and benchmarks. *Journal of Chemical Physics*, **2021**, 154, 084125	3.9	5
246	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021**, 97, 243-269	3.6	8
245	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
244	X-ray transient absorption reveals the A (nπ^*) state of pyrazine in electronic relaxation. *Nature Communications*, **2021**, 12, 5003	17.4	11
243	Calculation of spin-orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. *Journal of Chemical Physics*, **2020**, 153, 214107	3.9	12

242	Probing the Electronic Structure of Bulk Water at the Molecular Length Scale with Angle-Resolved Photoelectron Spectroscopy. *Journal of Physical Chemistry Letters*, **2020**, 11, 5162-5170	6.4	14
241	On the basis set selection for calculations of core-level states: different strategies to balance cost and accuracy. *Molecular Physics*, **2020**, 118, e1769872	1.7	21
240	Resonant Inelastic X-Ray Scattering Reveals Hidden Local Transitions of the Aqueous OH Radical. *Physical Review Letters*, **2020**, 124, 236001	7.4	18
239	Effective Hamiltonians derived from equation-of-motion coupled-cluster wave functions: Theory and application to the Hubbard and Heisenberg Hamiltonians. *Journal of Chemical Physics*, **2020**, 152, 094108	3.9	7
238	Long-Range N-N Bonding by Rydberg Electrons. *Journal of Physical Chemistry Letters*, **2020**, 11, 2284-2290	6.4	4
237	A simple molecular orbital picture of RIXS distilled from many-body damped response theory. *Journal of Chemical Physics*, **2020**, 152, 244118	3.9	11
236	Two Cycling Centers in One Molecule: Communication by Through-Bond Interactions and Entanglement of the Unpaired Electrons. *Journal of Physical Chemistry Letters*, **2020**, 11, 1297-1304	6.4	13
235	Extension of frozen natural orbital approximation to open-shell references: Theory, implementation, and application to single-molecule magnets. *Journal of Chemical Physics*, **2020**, 152, 034105	3.9	15
234	The quest to uncover the nature of benzonitrile anion. *Physical Chemistry Chemical Physics*, **2020**, 22, 5002-5010	3.6	4
233	Observation of the fastest chemical processes in the radiolysis of water. *Science*, **2020**, 367, 179-182	33.3	74
232	Spin-flip methods in quantum chemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 4326-4342	3.6	61
231	How to stay out of trouble in RIXS calculations within equation-of-motion coupled-cluster damped response theory? Safe hitchhiking in the excitation manifold by means of core-valence separation. *Physical Chemistry Chemical Physics*, **2020**, 22, 2629-2641	3.6	29
230	Dyson orbitals within the fc-CVS-EOM-CCSD framework: theory and application to X-ray photoelectron spectroscopy of ground and excited states. *Physical Chemistry Chemical Physics*, **2020**, 22, 2693-2703	3.6	27
229	Cherry-picking resolvents: A general strategy for convergent coupled-cluster damped response calculations of core-level spectra. *Journal of Chemical Physics*, **2020**, 153, 141104	3.9	6
228	Table-Top X-ray Spectroscopy of Benzene Radical Cation. *Journal of Physical Chemistry A*, **2020**, 124, 9524-9531	2.8	17
227	Toward Ultracold Organic Chemistry: Prospects of Laser Cooling Large Organic Molecules. *Journal of Physical Chemistry Letters*, **2020**, 11, 6670-6676	6.4	11
226	Interplay of Open-Shell Spin-Coupling and Jahn-Teller Distortion in Benzene Radical Cation Probed by X-ray Spectroscopy. *Journal of Physical Chemistry A*, **2020**, 124, 9532-9541	2.8	19
225	In search of molecular ions for optical cycling: a difficult road. *Physical Chemistry Chemical Physics*, **2020**, 22, 17075-17090	3.6	10

224	From orbitals to observables and back. *Journal of Chemical Physics*, **2020**, 153, 080901	3.9	40
223	Equation-of-Motion Coupled-Cluster Theory to Model L-Edge X-ray Absorption and Photoelectron Spectra. *Journal of Physical Chemistry Letters*, **2020**, 11, 8314-8321	6.4	23
222	The elusive dynamics of aqueous permanganate photochemistry. *Physical Chemistry Chemical Physics*, **2020**, 22, 10043-10055	3.6	4
221	Towards a rational design of laser-coolable molecules: insights from equation-of-motion coupled-cluster calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 19447-19457	3.6	20
220	Time-resolved near-edge X-ray absorption fine structure of pyrazine from electronic structure and nuclear wave packet dynamics simulations. *Journal of Chemical Physics*, **2019**, 151, 124114	3.9	23
219	EOM-CC guide to Fock-space travel: the C edition. *Faraday Discussions*, **2019**, 217, 514-532	3.6	11
218	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. *Journal of Physical Chemistry B*, **2019**, 123, 6133-6149	3.4	25
217	New and Efficient Equation-of-Motion Coupled-Cluster Framework for Core-Excited and Core-Ionized States. *Journal of Chemical Theory and Computation*, **2019**, 15, 3117-3133	6.4	86
216	To Be or Not To Be a Molecular Ion: The Role of the Solvent in Photoionization of Arginine. *Journal of Physical Chemistry Letters*, **2019**, 10, 1860-1865	6.4	4
215	Quantitative El-Sayed Rules for Many-Body Wave Functions from Spinless Transition Density Matrices. *Journal of Physical Chemistry Letters*, **2019**, 10, 4857-4862	6.4	23
214	Tribute to Hanna Reisler. *Journal of Physical Chemistry A*, **2019**, 123, 6381-6383	2.8	
213	General framework for calculating spin-orbit couplings using spinless one-particle density matrices: Theory and application to the equation-of-motion coupled-cluster wave functions. *Journal of Chemical Physics*, **2019**, 151, 034106	3.9	33
212	Triplet Excitons in Small Helium Clusters. *Journal of Physical Chemistry A*, **2019**, 123, 6113-6122	2.8	
211	Implementation of analytic gradients for CCSD and EOM-CCSD using Cholesky decomposition of the electron-repulsion integrals and their derivatives: Theory and benchmarks. *Journal of Chemical Physics*, **2019**, 151, 014110	3.9	17
210	Exotic systems: general discussion. *Faraday Discussions*, **2019**, 217, 601-622	3.6	
209	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. *Mendeleev Communications*, **2019**, 29, 187-189	1.9	6
208	Influence of the First Chromophore-Forming Residue on Photobleaching and Oxidative Photoconversion of EGFP and EYFP. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	5
207	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. *Journal of Physical Chemistry B*, **2019**, 123, 8901-8909	3.4	5

206	Spin-Forbidden Channels in Reactions of Unsaturated Hydrocarbons with O(P). *Journal of Physical Chemistry A*, **2019**, 123, 482-491	2.8	18
205	Distinct Electron Conductance Regimes in Bacterial Decaheme Cytochromes. *Angewandte Chemie - International Edition*, **2018**, 57, 6805-6809	16.4	17
204	Calculations of non-adiabatic couplings within equation-of-motion coupled-cluster framework: Theory, implementation, and validation against multi-reference methods. *Journal of Chemical Physics*, **2018**, 148, 044103	3.9	26
203	Singlet-triplet energy gaps and the degree of diradical character in binuclear copper molecular magnets characterized by spin-flip density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 13127-13144	3.6	36
202	Modeling Photoelectron Spectra of CuO, CuO, and CuO Anions with Equation-of-Motion Coupled-Cluster Methods: An Adventure in Fock Space. *Journal of Physical Chemistry A*, **2018**, 122, 3653-3664	2.8	10
201	Bound and continuum-embedded states of cyanopolyyne anions. *Physical Chemistry Chemical Physics*, **2018**, 20, 4805-4817	3.6	18
200	Characterizing Bonding Patterns in Diradicals and Triradicals by Density-Based Wave Function Analysis: A Uniform Approach. *Journal of Chemical Theory and Computation*, **2018**, 14, 638-648	6.4	29
199	Benchmarking Excited-State Calculations Using Exciton Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 710-725	6.4	97
198	Autocorrelation of electronic wave-functions: a new approach for describing the evolution of electronic structure in the course of dynamics. *Molecular Physics*, **2018**, 116, 2512-2523	1.7	1
197	Pyridinium Analogues of Green Fluorescent Protein Chromophore: Fluorogenic Dyes with Large Solvent-Dependent Stokes Shift. *Journal of Physical Chemistry Letters*, **2018**, 9, 1958-1963	6.4	25
196	Multiheme Cytochrome Mediated Redox Conduction through Shewanella oneidensis MR-1 Cells. *Journal of the American Chemical Society*, **2018**, 140, 10085-10089	16.4	48
195	Real and Imaginary Excitons: Making Sense of Resonance Wave Functions by Using Reduced State and Transition Density Matrices. *Journal of Physical Chemistry Letters*, **2018**, 9, 4101-4108	6.4	16
194	Linker-Dependent Singlet Fission in Tetracene Dimers. *Journal of the American Chemical Society*, **2018**, 140, 10179-10190	16.4	90
193	Vacuum ultraviolet photoionization cross section of the hydroxyl radical. *Journal of Chemical Physics*, **2018**, 148, 184302	3.9	15
192	Introduction: Theoretical Modeling of Excited State Processes. *Chemical Reviews*, **2018**, 118, 6925-6926	68.1	15
191	A Combined Experimental and Theoretical Study on the Formation of Interstellar Propylene Oxide (CH3CHCH2O)—A Chiral Molecule. *Astrophysical Journal*, **2018**, 860, 108	4.7	45
190	An ab Initio Exploration of the Bergman Cyclization. *Journal of Physical Chemistry A*, **2018**, 122, 420-430	2.8	10
189	The effect of polarizable environment on two-photon absorption cross sections characterized by the equation-of-motion coupled-cluster singles and doubles method combined with the effective fragment potential approach. *Journal of Chemical Physics*, **2018**, 149, 164109	3.9	14

188	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. *Journal of Chemical Physics*, **2018**, 149, 180901	3.9	49
187	Communication: The pole structure of the dynamical polarizability tensor in equation-of-motion coupled-cluster theory. *Journal of Chemical Physics*, **2018**, 149, 141101	3.9	9
186	Conversion of He(2 S) to He(a) in Liquid Helium. *Journal of Physical Chemistry Letters*, **2018**, 9, 6017-6023	6.4	4
185	Singlet Fission in Perylenediimide Dimers. *Journal of Physical Chemistry C*, **2018**, 122, 25753-25763	3.8	41
184	Distinct Electron Conductance Regimes in Bacterial Decaheme Cytochromes. *Angewandte Chemie*, **2018**, 130, 6921-6925	3.6	2
183	Double Precision Is Not Needed for Many-Body Calculations: Emergent Conventional Wisdom. *Journal of Chemical Theory and Computation*, **2018**, 14, 4088-4096	6.4	25
182	Electronic Structure and Rydberg-Core Interactions in Hydroxycarbene and Methylhydroxycarbene. *Journal of Physical Chemistry A*, **2018**, 122, 6176-6182	2.8	6
181	A General Sparse Tensor Framework for Electronic Structure Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 1108-1116	6.4	8
180	Rewriting the Story of Excimer Formation in Liquid Benzene. *Journal of Physical Chemistry A*, **2017**, 121, 1962-1975	2.8	22
179	The Quantum Chemistry of Open-Shell Species. *Reviews in Computational Chemistry*, **2017**, 151-224		35
178	Two-photon absorption spectroscopy of trans-stilbene, cis-stilbene, and phenanthrene: Theory and experiment. *Journal of Chemical Physics*, **2017**, 146, 144305	3.9	16
177	Two-photon absorption spectroscopy of stilbene and phenanthrene: Excited-state analysis and comparison with ethylene and toluene. *Journal of Chemical Physics*, **2017**, 146, 174102	3.9	16
176	Extending Quantum Chemistry of Bound States to Electronic Resonances. *Annual Review of Physical Chemistry*, **2017**, 68, 525-553	15.7	97
175	Effect of the diradical character on static polarizabilities and two-photon absorption cross sections: A closer look with spin-flip equation-of-motion coupled-cluster singles and doubles method. *Journal of Chemical Physics*, **2017**, 146, 224103	3.9	17
174	Cross-scale efficient tensor contractions for coupled cluster computations through multiple programming model backends. *Journal of Parallel and Distributed Computing*, **2017**, 106, 92-105	4.4	5
173	Photoelectron Spectroscopy Study of Quinonimides. *Journal of the American Chemical Society*, **2017**, 139, 11138-11148	16.4	14
172	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 10602-10609	3.4	6
171	Electronic Spectra of Tris(2,2N bipyridine)-M(II) Complex Ions in Vacuo (M = Fe and Os). *Inorganic Chemistry*, **2017**, 56, 7029-7037	5.1	12

170	Coupled-cluster based approach for core-level states in condensed phase: Theory and application to different protonated forms of aqueous glycine. *Journal of Chemical Physics*, **2017**, 147, 014107	3.9	31
169	Visualizing the Contributions of Virtual States to Two-Photon Absorption Cross Sections by Natural Transition Orbitals of Response Transition Density Matrices. *Journal of Physical Chemistry Letters*, **2017**, 8, 3256-3265	6.4	25
168	Molecular Modeling Clarifies the Mechanism of Chromophore Maturation in the Green Fluorescent Protein. *Journal of the American Chemical Society*, **2017**, 139, 10239-10249	16.4	31
167	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. *Chemical Reviews*, **2017**, 117, 758-795	53.1	154
166	Channel branching ratios in CHCN photodetachment: Rotational structure and vibrational energy redistribution in autodetachment. *Journal of Chemical Physics*, **2017**, 147, 234309	3.9	5
165	Probing Electronic Wave Functions of Sodium-Doped Clusters: Dyson Orbitals, Anisotropy Parameters, and Ionization Cross-Sections. *Journal of Physical Chemistry A*, **2016**, 120, 9841-9856	2.8	16
164	Extension of the Effective Fragment Potential Method to Macromolecules. *Journal of Physical Chemistry B*, **2016**, 120, 6562-74	3.4	65
163	Turning On and Off Photoinduced Electron Transfer in Fluorescent Proteins by π-Stacking, Halide Binding, and Tyr145 Mutations. *Journal of the American Chemical Society*, **2016**, 138, 4807-17	16.4	44
162	On couplings and excimers: lessons from studies of singlet fission in covalently linked tetracene dimers. *Physical Chemistry Chemical Physics*, **2016**, 18, 7751-61	3.6	81
161	Singlet Fission in a Covalently Linked Cofacial Alkynyltetracene Dimer. *Journal of the American Chemical Society*, **2016**, 138, 617-27	16.4	204
160	A study of interstellar aldehydes and enols as tracers of a cosmic ray-driven nonequilibrium synthesis of complex organic molecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7727-32	11.5	77
159	Reduced-cost sparsity-exploiting algorithm for solving coupled-cluster equations. *Journal of Computational Chemistry*, **2016**, 37, 1059-67	3.5	5
158	Quantifying local exciton, charge resonance, and multiexciton character in correlated wave functions of multichromophoric systems. *Journal of Chemical Physics*, **2016**, 144, 014102	3.9	28
157	Characterizing metastable states beyond energies and lifetimes: Dyson orbitals and transition dipole moments. *Journal of Chemical Physics*, **2016**, 144, 054113	3.9	45
156	Static polarizabilities for excited states within the spin-conserving and spin-flipping equation-of-motion coupled-cluster singles and doubles formalism: Theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2016**, 145, 204116	3.9	21
155	Intra- and Intermolecular Singlet Fission in Covalently Linked Dimers. *Journal of Physical Chemistry C*, **2016**, 120, 19070-19077	3.8	45
154	Same but Different: Dipole-Stabilized Shape Resonances in CuF(-) and AgF(.). *Journal of Physical Chemistry Letters*, **2015**, 6, 2786-93	6.4	43
153	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8

152	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. *Journal of Physical Chemistry B*, **2015**, 119, 5444-52	3.4	23
151	On the Nature of an Extended Stokes Shift in the mPlum Fluorescent Protein. *Journal of Physical Chemistry B*, **2015**, 119, 13052-62	3.4	24
150	Photoelectron wave function in photoionization: plane wave or Coulomb wave?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4532-40	6.4	97
149	Two-photon absorption cross sections within equation-of-motion coupled-cluster formalism using resolution-of-the-identity and Cholesky decomposition representations: Theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2015**, 142, 064118	3.9	48
148	Quantifying charge resonance and multiexciton character in coupled chromophores by charge and spin cumulant analysis. *Journal of Chemical Physics*, **2015**, 142, 224104	3.9	40
147	New algorithms for iterative matrix-free eigensolvers in quantum chemistry. *Journal of Computational Chemistry*, **2015**, 36, 273-84	3.5	34
146	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
145	Spin-orbit couplings within the equation-of-motion coupled-cluster framework: Theory, implementation, and benchmark calculations. *Journal of Chemical Physics*, **2015**, 143, 064102	3.9	68
144	The effects of resonance delocalization and the extent of □system on ionization energies of model fluorescent proteins chromophores. *International Journal of Quantum Chemistry*, **2015**, 115, 1258-1264	2.1	7
143	Ligand influence on the electronic spectra of monocationic copper-bipyridine complexes. *Physical Chemistry Chemical Physics*, **2015**, 17, 31938-46	3.6	29
142	Measurement of heavy ion energy at the test facility of electronic components. *Instruments and Experimental Techniques*, **2014**, 57, 11-16	0.5	2
141	Calculations predict a stable molecular crystal of N8. *Nature Chemistry*, **2014**, 6, 52-6	17.6	107
140	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 310-5	6.4	82
139	Complex Absorbing Potential Equation-of-Motion Coupled-Cluster Method Yields Smooth and Internally Consistent Potential Energy Surfaces and Lifetimes for Molecular Resonances. *Journal of Physical Chemistry Letters*, **2014**, 5, 3078-85	6.4	37
138	Dissecting the Effect of Morphology on the Rates of Singlet Fission: Insights from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 19608-19617	3.8	72
137	What we can learn from the norms of one-particle density matrices, and what we can□t: some results for interstate properties in model singlet fission systems. *Journal of Physical Chemistry A*, **2014**, 118, 11943-55	2.8	73
136	Complex absorbing potentials within EOM-CC family of methods: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2014**, 141, 024102	3.9	84
135	A Simple Kinetic Model for Singlet Fission: A Role of Electronic and Entropic Contributions to Macroscopic Rates. *Journal of Physical Chemistry C*, **2014**, 118, 5188-5195	3.8	103

134	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. *Journal of Chemical Theory and Computation*, **2014**, 10, 3074-84	6.4	132
133	Chromophore photoreduction in red fluorescent proteins is responsible for bleaching and phototoxicity. *Journal of Physical Chemistry B*, **2014**, 118, 4527-34	3.4	50
132	Analysis and tuning of libtensor framework on multicore architectures **2014**,		5
131	First-principles characterization of the energy landscape and optical spectra of green fluorescent protein along the A-kB proton transfer route. *Journal of the American Chemical Society*, **2013**, 135, 11541-9	13.4	55
130	New implementation of high-level correlated methods using a general block tensor library for high-performance electronic structure calculations. *Journal of Computational Chemistry*, **2013**, 34, 2293-2309	3.5	88
129	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 4495-506	6.4	76
128	Proton transfer in nucleobases is mediated by water. *Journal of Physical Chemistry A*, **2013**, 117, 6789-97	2.8	32
127	Fission of Entangled Spins: An Electronic Structure Perspective. *Journal of Physical Chemistry Letters*, **2013**, 4, 3845-3852	6.4	162
126	Photo-isomerization upshifts the pKa of the Photoactive Yellow Protein chromophore to contribute to photocycle propagation. *Journal of Photochemistry and Photobiology A: Chemistry*, **2013**, 270, 43-52	4.7	13
125	Complex-scaled equation-of-motion coupled-cluster method with single and double substitutions for autoionizing excited states: theory, implementation, and examples. *Journal of Chemical Physics*, **2013**, 138, 124106	3.9	55
124	Effective fragment potential method in Q-CHEM: a guide for users and developers. *Journal of Computational Chemistry*, **2013**, 34, 1060-70	3.5	44
123	Q-Chem: an engine for innovation. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 317-326	7.9	257
122	Toward organic photohydrides: excited-state behavior of 10-methyl-9-phenyl-9,10-dihydroacridine. *Journal of Physical Chemistry B*, **2013**, 117, 15290-6	3.4	15
121	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. *Journal of Physical Chemistry Letters*, **2013**, 4, 1743-7	6.4	25
120	On the photodetachment from the green fluorescent protein chromophore. *Journal of Physical Chemistry A*, **2013**, 117, 11815-22	2.8	31
119	Conical Intersection and Potential Energy Surface Features of a Model Retinal Chromophore: Comparison of EOM-CC and Multireference Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 284-92	6.4	62
118	General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: theory and benchmarks. *Journal of Chemical Physics*, **2013**, 139, 134105	3.9	94
117	Toward understanding the redox properties of model chromophores from the green fluorescent protein family: an interplay between conjugation, resonance stabilization, and solvent effects. *Journal of Physical Chemistry B*, **2012**, 116, 12398-405	3.4	18

116	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and Stacking on the Ionization Energy of Adenine in the AATT Tetramer. *Journal of Physical Chemistry Letters*, **2012**, 3, 2726-32	6.4	35
115	Electronic states of the benzene dimer: a simple case of complexity. *Journal of Physical Chemistry A*, **2012**, 116, 653-62	2.8	40
114	Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of hydrogen bonds. *Nature Chemistry*, **2012**, 4, 323-9	17.6	62
113	De-perturbative corrections for charge-stabilized double ionization potential equation-of-motion coupled-cluster method. *Journal of Chemical Physics*, **2012**, 136, 244109	3.9	20
112	Quantum chemistry behind bioimaging: insights from ab initio studies of fluorescent proteins and their chromophores. *Accounts of Chemical Research*, **2012**, 45, 265-75	24.3	114
111	Exploring structural and optical properties of fluorescent proteins by squeezing: modeling high-pressure effects on the mStrawberry and mCherry red fluorescent proteins. *Journal of Physical Chemistry B*, **2012**, 116, 12426-40	3.4	26
110	A VUV Photoionization and Ab Initio Determination of the Ionization Energy of a Gas-Phase Sugar (Deoxyribose). *Journal of Physical Chemistry Letters*, **2012**, 3, 97-101	6.4	38
109	First-principle protocol for calculating ionization energies and redox potentials of solvated molecules and ions: theory and application to aqueous phenol and phenolate. *Journal of Physical Chemistry B*, **2012**, 116, 7269-80	3.4	84
108	General formulation of spin-flip time-dependent density functional theory using non-collinear kernels: theory, implementation, and benchmarks. *Journal of Chemical Physics*, **2012**, 136, 204103	3.9	163
107	Insight into the common mechanism of the chromophore formation in the red fluorescent proteins: the elusive blue intermediate revealed. *Journal of the American Chemical Society*, **2012**, 134, 2807-14	16.4	36
106	Toward Molecular-Level Characterization of Photoinduced Decarboxylation of the Green Fluorescent Protein: Accessibility of the Charge-Transfer States. *Journal of Chemical Theory and Computation*, **2012**, 8, 1912-20	6.4	22
105	Overtone-induced dissociation and isomerization dynamics of the hydroxymethyl radical (CH2OH and CD2OH). I. A theoretical study. *Journal of Chemical Physics*, **2012**, 136, 084304	3.9	24
104	Effect of solvation on the vertical ionization energy of thymine: from microhydration to bulk. *Journal of Physical Chemistry A*, **2011**, 115, 6028-38	2.8	84
103	Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore. *Journal of Chemical Physics*, **2011**, 134, 034310	3.9	46
102	Non-Condon Effects in the One- and Two-Photon Absorption Spectra of the Green Fluorescent Protein. *Journal of Physical Chemistry Letters*, **2011**, 2, 488-492	6.4	63
101	Effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore. *Journal of Physical Chemistry B*, **2011**, 115, 8296-303	3.4	82
100	The effect of microhydration on ionization energies of thymine. *Faraday Discussions*, **2011**, 150, 313-30; discussion 391-418	3.6	38
99	Correction to What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?. *Journal of Physical Chemistry Letters*, **2011**, 2, 2695-2695	6.4	

98	Spectroscopy and fragmentation of undercoordinated bromoiridates. *Journal of Physical Chemistry A*, **2011**, 115, 13482-8	2.8	
97	What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?. *Journal of Physical Chemistry Letters*, **2011**, 2, 2593-2597	6.4	22
96	Effect of microhydration on the electronic structure of the chromophores of the photoactive yellow and green fluorescent proteins. *Journal of Chemical Physics*, **2011**, 135, 194304	3.9	28
95	Using the charge-stabilization technique in the double ionization potential equation-of-motion calculations with dianion references. *Journal of Chemical Physics*, **2011**, 135, 084109	3.9	46
94	Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism. *Journal of Chemical Physics*, **2010**, 132, 014109	3.9	85
93	Spectroscopic signatures of proton transfer dynamics in the water dimer cation. *Journal of Chemical Physics*, **2010**, 132, 194311	3.9	59
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