Anna I Krylov

List of Publications by Year
in descending order

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265 papers	22,314 citations	10979 71 h-index	10152 140 g-index
278 all docs	278 docs citations	278 times ranked	12895 citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Equation-of-Motion Coupled-Cluster Methods for Open-Shell and Electronically Excited Species: The Hitchhiker's Guide to Fock Space. Annual Review of Physical Chemistry, 2008, 59, 433-462.	4.8	830
4	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	1.5	617
5	The spinâ€“flip approach within time-dependent density functional theory: Theory and applications to diradicals. Journal of Chemical Physics, 2003, 118, 4807-4818.	1.2	581
6	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
7	Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model. Chemical Physics Letters, 2001, 338, 375-384.	1.2	430
8	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. Journal of Chemical Physics, 2002, 117, 4694-4708.	1.2	321
9	Equation-of-motion spin-flip coupled-cluster model with single and double substitutions: Theory and application to cyclobutadiene. Journal of Chemical Physics, 2004, 120, 175-185.	1.2	293
10	Qâ€Chem: an engine for innovation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 317-326.	6.2	287
11	Spin-Flip Equation-of-Motion Coupled-Cluster Electronic Structure Method for a Description of Excited States, Bond Breaking, Diradicals, and Triradicals. Accounts of Chemical Research, 2006, 39, 83-91.	7.6	275
12	Spin-flip configuration interaction: an electronic structure model that is both variational and size-consistent. Chemical Physics Letters, 2001, 350, 522-530.	1.2	254
13	Singlet Fission in a Covalently Linked Cofacial Alkynyltetracene Dimer. Journal of the American Chemical Society, 2016, 138, 617-627.	6.6	248
14	Dyson orbitals for ionization from the ground and electronically excited states within equation-of-motion coupled-cluster formalism: Theory, implementation, and examples. Journal of Chemical Physics, 2007, 127, 234106.	1.2	233
15	Energies and analytic gradients for a coupled-cluster doubles model using variational Brueckner orbitals: Application to symmetry breaking in O4+. Journal of Chemical Physics, 1998, 109, 4171-4181.	1.2	228
16	Size-consistent wave functions for nondynamical correlation energy: The valence active space optimized orbital coupled-cluster doubles model. Journal of Chemical Physics, 1998, 109, 10669-10678.	1.2	222
17	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. Chemical Reviews, 2017, 117, 758-795.	23.0	203
18	Perturbative corrections to the equation-of-motion spinâ€“flip self-consistent field model: Application to bond-breaking and equilibrium properties of diradicals. Journal of Chemical Physics, 2002, 116, 3194-3203.	1.2	192

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19	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.	1.2	188
20	Fission of Entangled Spins: An Electronic Structure Perspective. Journal of Physical Chemistry Letters, 2013, 4, 3845-3852.	2.1	170
21	Cross sections and photoelectron angular distributions in photodetachment from negative ions using equation-of-motion coupled-cluster Dyson orbitals. Journal of Chemical Physics, 2009, 131, 124114.	1.2	165
22	Femtosecond Multidimensional Imaging of a Molecular Dissociation. Science, 2006, 311, 219-222.	6.0	164
23	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, 3074-3084.	2.3	161
24	Second-order perturbation corrections to singles and doubles coupled-cluster methods: General theory and application to the valence optimized doubles model. Journal of Chemical Physics, 2000, 113, 3548-3560.	1.2	155
25	Calculations predict a stable molecular crystal of N8. Nature Chemistry, 2014, 6, 52-56.	6.6	152
26	Observation of the fastest chemical processes in the radiolysis of water. Science, 2020, 367, 179-182.	6.0	149
27	A spin-complete version of the spin-flip approach to bond breaking: What is the impact of obtaining spin eigenfunctions?. Journal of Chemical Physics, 2003, 118, 9084-9094.	1.2	142
28	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.	2.3	139
29	A noniterative perturbative triples correction for the spin-flipping and spin-conserving equation-of-motion coupled-cluster methods with single and double substitutions. Journal of Chemical Physics, 2008, 129, 194105.	1.2	138
30	Extending Quantum Chemistry of Bound States to Electronic Resonances. Annual Review of Physical Chemistry, 2017, 68, 525-553.	4.8	136
31	Linker-Dependent Singlet Fission in Tetracene Dimers. Journal of the American Chemical Society, 2018, 140, 10179-10190.	6.6	129
32	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	2.3	128
33	Excited states theory for optimized orbitals and valence optimized orbitals coupled-cluster doubles models. Journal of Chemical Physics, 2000, 113, 6509-6527.	1.2	125
34	Quantum Chemistry Behind Bioimaging: Insights from Ab Initio Studies of Fluorescent Proteins and Their Chromophores. Accounts of Chemical Research, 2012, 45, 265-275.	7.6	125
35	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.	1.2	117
36	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.	1.5	116

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37	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	1.1	115
38	Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?. Journal of Physical Chemistry Letters, 2015, 6, 4532-4540.	2.1	115
39	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, 7269-7280.	1.2	113
40	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	1.2	113
41	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. Journal of Chemical Theory and Computation, 2009, 5, 1895-1906.	2.3	109
42	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. Journal of Chemical Physics, 2005, 123, 084107.	1.2	107
43	Potential Energy Landscape of the Electronic States of the GFP Chromophore in Different Protonation Forms: Electronic Transition Energies and Conical Intersections. Journal of Chemical Theory and Computation, 2010, 6, 2377-2387.	2.3	106
44	New implementation of highâ€level correlated methods using a general block tensor library for highâ€performance electronic structure calculations. Journal of Computational Chemistry, 2013, 34, 2293-2309.	1.5	105
45	Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism. Journal of Chemical Physics, 2010, 132, 014109.	1.2	103
46	Spin-flip methods in quantum chemistry. Physical Chemistry Chemical Physics, 2020, 22, 4326-4342.	1.3	102
47	Noncovalent Interactions in Extended Systems Described by the Effective Fragment Potential Method: Theory and Application to Nucleobase Oligomers. Journal of Physical Chemistry A, 2010, 114, 12739-12754.	1.1	100
48	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. Journal of Physical Chemistry Letters, 2014, 5, 310-315.	2.1	99
49	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, 7727-7732.	3.3	99
50	Interacting Rydberg and valence states in radicals and molecules: experimental and theoretical studies. International Reviews in Physical Chemistry, 2009, 28, 267-308.	0.9	95
51	Effect of Solvation on the Vertical Ionization Energy of Thymine: From Microhydration to Bulk. Journal of Physical Chemistry A, 2011, 115, 6028-6038.	1.1	95
52	Products of the Benzene + O(³P) Reaction. Journal of Physical Chemistry A, 2010, 114, 3355-3370.	1.1	92
53	On couplings and excimers: lessons from studies of singlet fission in covalently linked tetracene dimers. Physical Chemistry Chemical Physics, 2016, 18, 7751-7761.	1.3	92
54	Electronic Structure and Spectroscopy of Nucleic Acid Bases: Ionization Energies, Ionization-Induced Structural Changes, and Photoelectron Spectra. Journal of Physical Chemistry A, 2010, 114, 12305-12317.	1.1	91

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55	Electronic structure of the trimethylenemethane diradical in its ground and electronically excited states:â€,Bonding, equilibrium geometries, and vibrational frequencies. Journal of Chemical Physics, 2003, 118, 6874-6883.	1.2	90
56	Multiheme Cytochrome Mediated Redox Conduction through Shewanella oneidensis MR-1 Cells. Journal of the American Chemical Society, 2018, 140, 10085-10089.	6.6	89
57	Charge localization and Jahnâ€“Teller distortions in the benzene dimer cation. Journal of Chemical Physics, 2008, 129, 074104.	1.2	88
58	The effect of Ï€-stacking, H-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenineâ€“adenine, thymineâ€“thymine and adenineâ€“thymine dimers. Physical Chemistry Chemical Physics, 2010, 12, 2292.	1.3	88
59	Spin-contamination of coupled-cluster wave functions. Journal of Chemical Physics, 2000, 113, 6052-6062.	1.2	87
60	Triradicals. Journal of Physical Chemistry A, 2005, 109, 10638-10645.	1.1	87
61	Effect of Protein Environment on Electronically Excited and Ionized States of the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry B, 2011, 115, 8296-8303.	1.2	87
62	Double spin-flip approach within equation-of-motion coupled cluster and configuration interaction formalisms: Theory, implementation, and examples. Journal of Chemical Physics, 2009, 130, 044103.	1.2	86
63	Benchmark full configuration interaction and equation-of-motion coupled-cluster model with single and double substitutions for ionized systems results for prototypical charge transfer systems: Noncovalent ionized dimers. Journal of Chemical Physics, 2007, 127, 164110.	1.2	85
64	Electronic Structure of the Water Dimer Cation. Journal of Physical Chemistry A, 2008, 112, 6159-6170.	1.1	84
65	From orbitals to observables and back. Journal of Chemical Physics, 2020, 153, 080901.	1.2	84
66	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, 4495-4506.	2.3	83
67	Analytic gradients for the spin-conserving and spin-flipping equation-of-motion coupled-cluster models with single and double substitutions. Journal of Chemical Physics, 2005, 122, 224106.	1.2	82
68	Dissecting the Effect of Morphology on the Rates of Singlet Fission: Insights from Theory. Journal of Physical Chemistry C, 2014, 118, 19608-19617.	1.5	80
69	What We Can Learn from the Norms of One-Particle Density Matrices, and What We Canâ€™t: Some Results for Interstate Properties in Model Singlet Fission Systems. Journal of Physical Chemistry A, 2014, 118, 11943-11955.	1.1	80
70	Spin-orbit couplings within the equation-of-motion coupled-cluster framework: Theory, implementation, and benchmark calculations. Journal of Chemical Physics, 2015, 143, 064102.	1.2	80
71	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.	2.1	77
72	Extension of the Effective Fragment Potential Method to Macromolecules. Journal of Physical Chemistry B, 2016, 120, 6562-6574.	1.2	72

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73	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
74	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, 284-292.	2.3	70
75	Bonding Patterns in Benzene Triradicals from Structural, Spectroscopic, and Thermochemical Perspectives. Journal of Physical Chemistry A, 2004, 108, 6581-6588.	1.1	69
76	Spectroscopic signatures of proton transfer dynamics in the water dimer cation. Journal of Chemical Physics, 2010, 132, 194311.	1.2	69
77	Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of hydrogen bonds. Nature Chemistry, 2012, 4, 323-329.	6.6	69
78	The <scp>ezSpectra</scp> suite: An easyâ€toâ€use toolkit for spectroscopy modeling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1546.	6.2	67
79	Ionization of cytosine monomer and dimer studied by VUV photoionization and electronic structure calculations. Physical Chemistry Chemical Physics, 2010, 12, 2860.	1.3	65
80	First-Principles Characterization of the Energy Landscape and Optical Spectra of Green Fluorescent Protein along the Aâ†'Iâ†'B Proton Transfer Route. Journal of the American Chemical Society, 2013, 135, 11541-11549.	6.6	64
81	Singlet Fission in Perylenediimide Dimers. Journal of Physical Chemistry C, 2018, 122, 25753-25763.	1.5	64
82	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.	1.2	63
83	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.	1.2	63
84	Photodissociation dynamics of HCl in solid Ar: Cage exit, nonadiabatic transitions, and recombination. Journal of Chemical Physics, 1997, 106, 6574-6587.	1.2	62
85	Roaming Pathway Leading to Unexpected Water + Vinyl Products in C₂H₄OH Dissociation. Journal of Physical Chemistry Letters, 2010, 1, 3058-3065.	2.1	62
86	Electronic structure of the benzene dimer cation. Journal of Chemical Physics, 2007, 127, 044317.	1.2	61
87	Electronic structure of the 1,3,5-tridehydrobenzene triradical in its ground and excited states. Journal of Chemical Physics, 2003, 118, 9614-9622.	1.2	59
88	5-Dehydro-1,3-quinodimethane: A Hydrocarbon with an Open-Shell Doublet Ground State. Angewandte Chemie - International Edition, 2004, 43, 742-745.	7.2	58
89	Characterizing metastable states beyond energies and lifetimes: Dyson orbitals and transition dipole moments. Journal of Chemical Physics, 2016, 144, 054113.	1.2	58
90	Intra- and Intermolecular Singlet Fission in Covalently Linked Dimers. Journal of Physical Chemistry C, 2016, 120, 19070-19077.	1.5	56

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91	Chromophore Photoreduction in Red Fluorescent Proteins Is Responsible for Bleaching and Phototoxicity. Journal of Physical Chemistry B, 2014, 118, 4527-4534.	1.2	55
92	Same but Different: Dipole-Stabilized Shape Resonances in CuF^{â€“} and AgF^{â€“}. Journal of Physical Chemistry Letters, 2015, 6, 2786-2793.	2.1	55
93	Nonadiabatic dynamics and electronic energy relaxation of Cl(2P) atoms in solid Ar. Journal of Chemical Physics, 1996, 105, 4626-4635.	1.2	54
94	A Combined Experimental and Theoretical Study on the Formation of Interstellar Propylene Oxide (CH₃CHCH₂O)â€”A Chiral Molecule. Astrophysical Journal, 2018, 860, 108.	1.6	54
95	Photodissociation of ICN in solid and in liquid Ar: Dynamics of the cage effect and of excitedâ€state isomerization. Journal of Chemical Physics, 1994, 100, 4242-4252.	1.2	52
96	Turning On and Off Photoinduced Electron Transfer in Fluorescent Proteins by Ï€-Stacking, Halide Binding, and Tyr145 Mutations. Journal of the American Chemical Society, 2016, 138, 4807-4817.	6.6	52
97	New algorithm for tensor contractions on multi-core CPUs, GPUs, and accelerators enables CCSD and EOM-CCSD calculations with over 1000 basis functions on a single compute node. Journal of Computational Chemistry, 2017, 38, 842-853.	1.5	51
98	Perturbative triples correction for the equation-of-motion coupled-cluster wave functions with single and double substitutions for ionized states: Theory, implementation, and examples. Journal of Chemical Physics, 2009, 131, 114112.	1.2	50
99	Using the charge-stabilization technique in the double ionization potential equation-of-motion calculations with dianion references. Journal of Chemical Physics, 2011, 135, 084109.	1.2	49
100	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, 3078-3085.	2.1	48
101	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.	1.3	48
102	The effect of Ï€-stacking and H-bonding on ionization energies of a nucleobase: uracil dimer cation. Physical Chemistry Chemical Physics, 2009, 11, 1303.	1.3	47
103	Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore. Journal of Chemical Physics, 2011, 134, 034310.	1.2	47
104	Effective fragment potential method in <scp>Qâ€CHEM</scp>: A guide for users and developers. Journal of Computational Chemistry, 2013, 34, 1060-1070.	1.5	47
105	Quantifying charge resonance and multiexciton character in coupled chromophores by charge and spin cumulant analysis. Journal of Chemical Physics, 2015, 142, 224104.	1.2	46
106	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.	2.1	46
107	Singletâ€“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.	1.3	45
108	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. Cisâ^’Trans Isomerization in Water. Journal of Chemical Theory and Computation, 2009, 5, 1907-1914.	2.3	44

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109	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.	1.2	44
110	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and Ï€-Stacking on the Ionization Energy of Adenine in the AATT Tetramer. Journal of Physical Chemistry Letters, 2012, 3, 2726-2732.	2.1	43
111	Electronic States of the Benzene Dimer: A Simple Case of Complexity. Journal of Physical Chemistry A, 2012, 116, 653-662.	1.1	43
112	Proton Transfer in Nucleobases is Mediated by Water. Journal of Physical Chemistry A, 2013, 117, 6789-6797.	1.1	43
113	New algorithms for iterative matrixâ€free eigensolvers in quantum chemistry. Journal of Computational Chemistry, 2015, 36, 273-284.	1.5	43
114	Conical and glancing Jahn-Teller intersections in the cyclic trinitrogen cation. Journal of Chemical Physics, 2006, 124, 224309.	1.2	42
115	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 coreâ€“valence separation. Physical Chemistry Chemical Physics, 2020, 22, 2629-2641.	1.3	42
116	The effect of substituents on electronic statesâ€™ ordering in meta-xylylene diradicals: Qualitative insights from quantitative studies. Journal of Chemical Physics, 2005, 123, 104304.	1.2	41
117	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.	2.1	41
118	Quantitative El-Sayed Rules for Many-Body Wave Functions from Spinless Transition Density Matrices. Journal of Physical Chemistry Letters, 2019, 10, 4857-4862.	2.1	41
119	General framework for calculating spinâ€“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.	1.2	41
120	Photodissociation of HCl adsorbed on the surface of an Ar12 cluster: Nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1999, 110, 11047-11053.	1.2	40
121	Molecular Modeling Clarifies the Mechanism of Chromophore Maturation in the Green Fluorescent Protein. Journal of the American Chemical Society, 2017, 139, 10239-10249.	6.6	39
122	On the basis set selection for calculations of core-level states: different strategies to balance cost and accuracy. Molecular Physics, 2020, 118, e1769872.	0.8	39
123	Photodissociation, electronic relaxation and recombination of HCl in Arn(HCl) clusters Non-adiabatic molecular dynamics simulations. Faraday Discussions, 1997, 108, 243-254.	1.6	38
124	The Role of Excited-State Topology in Three-Body Dissociation of sym -Triazine. Science, 2008, 321, 826-830.	6.0	38
125	Quantum Chemistry Calculations Provide Support to the Mechanism of the Light-Induced Structural Changes in the Flavin-Binding Photoreceptor Proteins. Journal of Chemical Theory and Computation, 2010, 6, 2293-2302.	2.3	38
126	The effect of microhydration on ionization energies of thymine. Faraday Discussions, 2011, 150, 313.	1.6	38

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127	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, 2807-2814.	6.6	38
128	Double Precision Is Not Needed for Many-Body Calculations: Emergent Conventional Wisdom. Journal of Chemical Theory and Computation, 2018, 14, 4088-4096.	2.3	38
129	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. Journal of Physical Chemistry B, 2019, 123, 6133-6149.	1.2	38
130	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.	1.2	37
131	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.	2.1	37
132	Pyridinium Analogues of Green Fluorescent Protein Chromophore: Fluorogenic Dyes with Large Solvent-Dependent Stokes Shift. Journal of Physical Chemistry Letters, 2018, 9, 1958-1963.	2.1	37
133	Towards a rational design of laser-coolable molecules: insights from equation-of-motion coupled-cluster calculations. Physical Chemistry Chemical Physics, 2019, 21, 19447-19457.	1.3	36
134	Degree of Initial Hole Localization/Delocalization in Ionized Water Clusters. Journal of Physical Chemistry A, 2009, 113, 4423-4429.	1.1	35
135	On the Nature of an Extended Stokes Shift in the mPlum Fluorescent Protein. Journal of Physical Chemistry B, 2015, 119, 13052-13062.	1.2	35
136	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.	2.3	35
137	Photodissociation Dynamics of Formaldehyde Initiated at the T₁/S₀ Minimum Energy Crossing Configurations. Journal of Physical Chemistry A, 2008, 112, 13267-13270.	1.1	34
138	On the Photodetachment from the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry A, 2013, 117, 11815-11822.	1.1	34
139	The theoretical prediction of infrared spectra of trans- and cis-hydroxycarbene calculated using full dimensional ab initio potential energy and dipole moment surfaces. Journal of Chemical Physics, 2008, 128, 204310.	1.2	33
140	Spectroscopy, polarization and nonadiabatic dynamics of electronically excited Ba(Ar)n clusters: Theory and experiment. Journal of Chemical Physics, 1996, 104, 3651-3663.	1.2	32
141	The 1,2,3-Tridehydrobenzene Triradical:â€‰ 2B or Not 2B? The Answer is 2A!. Journal of Physical Chemistry A, 2007, 111, 5071-5080.	1.1	32
142	A new electronic structure method for doublet states: Configuration interaction in the space of ionized 1h and 2h1p determinants. Journal of Chemical Physics, 2009, 130, 124113.	1.2	32
143	The effect of oxidation on the electronic structure of the green fluorescent protein chromophore. Journal of Chemical Physics, 2010, 132, 115104.	1.2	32
144	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, 12426-12440.	1.2	32

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145	Ligand influence on the electronic spectra of monocationic copperâ€“bipyridine complexes. Physical Chemistry Chemical Physics, 2015, 17, 31938-31946.	1.3	32
146	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.	1.2	32
147	Performance of the Spin-Flip and Multireference Methods for Bond Breaking in Hydrocarbons:â€‰ A Benchmark Study. Journal of Physical Chemistry A, 2007, 111, 13264-13271.	1.1	31
148	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.	1.2	31
149	Interplay of Open-Shell Spin-Coupling and Jahnâ€“Teller Distortion in Benzene Radical Cation Probed by X-ray Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 9532-9541.	1.1	31
150	The photoelectron spectrum of elusive cyclic-N3 and characterization of the potential energy surface and vibrational states of the ion. Journal of Chemical Physics, 2006, 125, 084306.	1.2	30
151	Quantifying local exciton, charge resonance, and multiexciton character in correlated wave functions of multichromophoric systems. Journal of Chemical Physics, 2016, 144, 014102.	1.2	30
152	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.	1.2	30
153	X-ray transient absorption reveals the 1Au (nÏ€*) state of pyrazine in electronic relaxation. Nature Communications, 2021, 12, 5003.	5.8	29
154	Photodissociation dynamics of the NO dimer. I. Theoretical overview of the ultraviolet singlet excited states. Journal of Chemical Physics, 2006, 125, 084301.	1.2	28
155	Electronic Structure of Carbon Trioxide and Vibronic Interactions Involving Jahnâ^'Teller States. Journal of Physical Chemistry A, 2007, 111, 8271-8276.	1.1	28
156	Ab Initio Calculation of the Photoelectron Spectra of the Hydroxycarbene Diradicals. Journal of Physical Chemistry A, 2009, 113, 7802-7809.	1.1	28
157	Electronic Structure and Spectroscopy of Oxyallyl: A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 6935-6943.	1.1	28
158	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. Journal of Physical Chemistry B, 2015, 119, 5444-5452.	1.2	28
159	Rewriting the Story of Excimer Formation in Liquid Benzene. Journal of Physical Chemistry A, 2017, 121, 1962-1975.	1.1	28
160	Two-photon absorption spectroscopy of trans-stilbene, cis-stilbene, and phenanthrene: Theory and experiment. Journal of Chemical Physics, 2017, 146, 144305.	1.2	28
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