Anna I Krylov

List of Publications by Year
in descending order

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265 papers	22,314 citations	12597 71 h-index	11608 140 g-index
278 all docs	278 docs citations	278 times ranked	14590 citing authors

#	Article	IF	Citations
1	Magnetic exchange interactions in binuclear and tetranuclear iron(III) complexes described by spinâ€flip DFT and Heisenberg effective Hamiltonians. Journal of Computational Chemistry, 2023, 44, 367-380.	1.5	9
2	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
3	Royal Society of Chemistry Provides Guidelines for Censorship to its Editors. Chemistry International, 2022, 44, 32-34.	0.3	4
4	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	16
5	Scientists must resist cancel culture. Nachrichten Aus Der Chemie, 2022, 70, 12-14.	0.0	6
6	Probing Molecular Chirality of Ground and Electronically Excited States in the UVâ€“vis and X-ray Regimes: An EOM-CCSD Study. Journal of Chemical Theory and Computation, 2022, 18, 1748-1764.	2.3	12
7	How Reproducible Are QM/MM Simulations? Lessons from Computational Studies of the Covalent Inhibition of the SARS-CoV-2 Main Protease by Carmofur. Journal of Chemical Theory and Computation, 2022, 18, 5056-5067.	2.3	9
8	Photoelectron photofragment coincidence spectroscopy of aromatic carboxylates: benzoate and p-coumarate. Physical Chemistry Chemical Physics, 2021, 23, 18414-18424.	1.3	5
9	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.	1.2	13
10	Feshbachâ€“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.	1.2	24
11	Feshbachâ€“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.	1.2	19
12	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	1.3	26
13	Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2021, 154, 114115.	1.2	17
14	An assessment of different electronic structure approaches for modeling time-resolved x-ray absorption spectroscopy. Structural Dynamics, 2021, 8, 024101.	0.9	18
15	Is Solid Copper Oxalate a Spin Chain or a Mixture of Entangled Spin Pairs?. Journal of Physical Chemistry C, 2021, 125, 7502-7510.	1.5	11
16	The orbital picture of the first dipole hyperpolarizability from many-body response theory. Journal of Chemical Physics, 2021, 154, 184109.	1.2	7
17	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.	2.3	12
18	The Peril of Politicizing Science. Journal of Physical Chemistry Letters, 2021, 12, 5371-5376.	2.1	12

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19	The Middle Science: Traversing Scale In Complex Many-Body Systems. ACS Central Science, 2021, 7, 1271-1287.	5.3	16
20	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
21	X-ray transient absorption reveals the 1Au (nÏ€*) state of pyrazine in electronic relaxation. Nature Communications, 2021, 12, 5003.	5.8	29
22	Quantum computing and quantum information storage. Physical Chemistry Chemical Physics, 2021, 23, 6341-6343.	1.3	4
23	Role of the Electronâ€“Dipole Interaction in Photodetachment Angular Distributions. Journal of Physical Chemistry Letters, 2021, 12, 10086-10092.	2.1	7
24	Observation of the fastest chemical processes in the radiolysis of water. Science, 2020, 367, 179-182.	6.0	149
25	Spin-flip methods in quantum chemistry. Physical Chemistry Chemical Physics, 2020, 22, 4326-4342.	1.3	102
26	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
27	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
28	Cherry-picking resolvents: A general strategy for convergent coupled-cluster damped response calculations of core-level spectra. Journal of Chemical Physics, 2020, 153, 141104.	1.2	13
29	Table-Top X-ray Spectroscopy of Benzene Radical Cation. Journal of Physical Chemistry A, 2020, 124, 9524-9531.	1.1	24
30	Toward Ultracold Organic Chemistry: Prospects of Laser Cooling Large Organic Molecules. Journal of Physical Chemistry Letters, 2020, 11, 6670-6676.	2.1	26
31	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
32	In search of molecular ions for optical cycling: a difficult road. Physical Chemistry Chemical Physics, 2020, 22, 17075-17090.	1.3	20
33	From orbitals to observables and back. Journal of Chemical Physics, 2020, 153, 080901.	1.2	84
34	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
35	Calculation of spinâ€“orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. Journal of Chemical Physics, 2020, 153, 214107.	1.2	18
36	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.	2.1	27

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37	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
38	Resonant Inelastic X-Ray Scattering Reveals Hidden Local Transitions of the Aqueous OH Radical. Physical Review Letters, 2020, 124, 236001.	2.9	28
39	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.	1.2	14
40	Long-Range Nâ€“N Bonding by Rydberg Electrons. Journal of Physical Chemistry Letters, 2020, 11, 2284-2290.	2.1	8
41	A simple molecular orbital picture of RIXS distilled from many-body damped response theory. Journal of Chemical Physics, 2020, 152, 244118.	1.2	20
42	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.	2.1	25
43	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.	1.2	27
44	The quest to uncover the nature of benzonitrile anion. Physical Chemistry Chemical Physics, 2020, 22, 5002-5010.	1.3	14
45	The elusive dynamics of aqueous permanganate photochemistry. Physical Chemistry Chemical Physics, 2020, 22, 10043-10055.	1.3	7
46	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
47	Tribute to Hanna Reisler. Journal of Physical Chemistry A, 2019, 123, 6381-6383.	1.1	0
48	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
49	Triplet Excitons in Small Helium Clusters. Journal of Physical Chemistry A, 2019, 123, 6113-6122.	1.1	1
50	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.	1.2	27
51	Exotic systems: general discussion. Faraday Discussions, 2019, 217, 601-622.	1.6	0
52	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. Mendeleev Communications, 2019, 29, 187-189.	0.6	8
53	Influence of the First Chromophore-Forming Residue on Photobleaching and Oxidative Photoconversion of EGFP and EYFP. International Journal of Molecular Sciences, 2019, 20, 5229.	1.8	18
54	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. Journal of Physical Chemistry B, 2019, 123, 8901-8909.	1.2	11

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55	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
56	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
57	EOM-CC guide to Fock-space travel: the C₂ edition. Faraday Discussions, 2019, 217, 514-532.	1.6	15
58	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
59	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
60	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.	2.1	6
61	Spin-Forbidden Channels in Reactions of Unsaturated Hydrocarbons with O(³P). Journal of Physical Chemistry A, 2019, 123, 482-491.	1.1	20
62	Distinct Electron Conductance Regimes in Bacterial Decaheme Cytochromes. Angewandte Chemie - International Edition, 2018, 57, 6805-6809.	7.2	27
63	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
64	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
65	Modeling Photoelectron Spectra of CuO, Cu₂O, and CuO₂ Anions with Equation-of-Motion Coupled-Cluster Methods: An Adventure in Fock Space. Journal of Physical Chemistry A, 2018, 122, 3653-3664.	1.1	12
66	Bound and continuum-embedded states of cyanopolyyne anions. Physical Chemistry Chemical Physics, 2018, 20, 4805-4817.	1.3	27
67	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
68	Benchmarking Excited-State Calculations Using Exciton Properties. Journal of Chemical Theory and Computation, 2018, 14, 710-725.	2.3	128
69	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.	0.8	2
70	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
71	An ab Initio Exploration of the Bergman Cyclization. Journal of Physical Chemistry A, 2018, 122, 420-430.	1.1	16
72	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.	1.2	20

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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	Communication: The pole structure of the dynamical polarizability tensor in equation-of-motion coupled-cluster theory. Journal of Chemical Physics, 2018, 149, 141101.	1.2	14
75	Conversion of He(2³S) to He₂(a³Î£_u⁺) in Liquid Helium. Journal of Physical Chemistry Letters, 2018, 9, 6017-6023.	2.1	4
76	Singlet Fission in Perylenediimide Dimers. Journal of Physical Chemistry C, 2018, 122, 25753-25763.	1.5	64
77	Distinct Electron Conductance Regimes in Bacterial Decaheme Cytochromes. Angewandte Chemie, 2018, 130, 6921-6925.	1.6	3
78	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
79	Electronic Structure and Rydbergâ€“Core Interactions in Hydroxycarbene and Methylhydroxycarbene. Journal of Physical Chemistry A, 2018, 122, 6176-6182.	1.1	7
80	Multiheme Cytochrome Mediated Redox Conduction through Shewanella oneidensis MR-1 Cells. Journal of the American Chemical Society, 2018, 140, 10085-10089.	6.6	89
81	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.	2.1	22
82	Linker-Dependent Singlet Fission in Tetracene Dimers. Journal of the American Chemical Society, 2018, 140, 10179-10190.	6.6	129
83	Vacuum ultraviolet photoionization cross section of the hydroxyl radical. Journal of Chemical Physics, 2018, 148, 184302.	1.2	20
84	Introduction: Theoretical Modeling of Excited State Processes. Chemical Reviews, 2018, 118, 6925-6926.	23.0	20
85	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
86	A General Sparse Tensor Framework for Electronic Structure Theory. Journal of Chemical Theory and Computation, 2017, 13, 1108-1116.	2.3	10
87	Rewriting the Story of Excimer Formation in Liquid Benzene. Journal of Physical Chemistry A, 2017, 121, 1962-1975.	1.1	28
88	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
89	Two-photon absorption spectroscopy of trans-stilbene, cis-stilbene, and phenanthrene: Theory and experiment. Journal of Chemical Physics, 2017, 146, 144305.	1.2	28
90	Two-photon absorption spectroscopy of stilbene and phenanthrene: Excited-state analysis and comparison with ethylene and toluene. Journal of Chemical Physics, 2017, 146, 174102.	1.2	20

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91	Extending Quantum Chemistry of Bound States to Electronic Resonances. Annual Review of Physical Chemistry, 2017, 68, 525-553.	4.8	136
92	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.	1.2	20
93	Cross-scale efficient tensor contractions for coupled cluster computations through multiple programming model backends. Journal of Parallel and Distributed Computing, 2017, 106, 92-105.	2.7	6
94	Photoelectron Spectroscopy Study of Quinonimides. Journal of the American Chemical Society, 2017, 139, 11138-11148.	6.6	18
95	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. Journal of Physical Chemistry B, 2017, 121, 10602-10609.	1.2	8
96	Electronic Spectra of Tris(2,2â€²-bipyridine)-M(II) Complex Ions in Vacuo (M = Fe and Os). Inorganic Chemistry, 2017, 56, 7029-7037.	1.9	14
97	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
98	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
99	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
100	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. Chemical Reviews, 2017, 117, 758-795.	23.0	203
101	Channel branching ratios in CH2CNâ^' photodetachment: Rotational structure and vibrational energy redistribution in autodetachment. Journal of Chemical Physics, 2017, 147, 234309.	1.2	9
102	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
103	Reducedâ€cost sparsityâ€exploiting algorithm for solving coupledâ€cluster equations. Journal of Computational Chemistry, 2016, 37, 1059-1067.	1.5	5
104	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
105	Characterizing metastable states beyond energies and lifetimes: Dyson orbitals and transition dipole moments. Journal of Chemical Physics, 2016, 144, 054113.	1.2	58
106	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
107	Intra- and Intermolecular Singlet Fission in Covalently Linked Dimers. Journal of Physical Chemistry C, 2016, 120, 19070-19077.	1.5	56
108	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.	1.1	20

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109	Extension of the Effective Fragment Potential Method to Macromolecules. Journal of Physical Chemistry B, 2016, 120, 6562-6574.	1.2	72
110	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
111	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
112	Singlet Fission in a Covalently Linked Cofacial Alkynyltetracene Dimer. Journal of the American Chemical Society, 2016, 138, 617-627.	6.6	248
113	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
114	The effects of resonance delocalization and the extent of Ï€ system on ionization energies of model fluorescent proteins chromophores. International Journal of Quantum Chemistry, 2015, 115, 1258-1264.	1.0	7
115	Ligand influence on the electronic spectra of monocationic copperâ€“bipyridine complexes. Physical Chemistry Chemical Physics, 2015, 17, 31938-31946.	1.3	32
116	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
117	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	2.1	19
118	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
119	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
120	Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?. Journal of Physical Chemistry Letters, 2015, 6, 4532-4540.	2.1	115
121	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
122	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
123	New algorithms for iterative matrixâ€free eigensolvers in quantum chemistry. Journal of Computational Chemistry, 2015, 36, 273-284.	1.5	43
124	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
125	Analysis and tuning of libtensor framework on multicore architectures. , 2014, , .		7
126	Measurement of heavy ion energy at the test facility of electronic components. Instruments and Experimental Techniques, 2014, 57, 11-16.	0.1	3

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127	Calculations predict a stable molecular crystal of N8. Nature Chemistry, 2014, 6, 52-56.	6.6	152
128	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
129	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
130	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
131	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
132	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	1.2	113
133	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
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, 3074-3084.	2.3	161
135	Chromophore Photoreduction in Red Fluorescent Proteins Is Responsible for Bleaching and Phototoxicity. Journal of Physical Chemistry B, 2014, 118, 4527-4534.	1.2	55
136	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
137	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
138	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
139	Proton Transfer in Nucleobases is Mediated by Water. Journal of Physical Chemistry A, 2013, 117, 6789-6797.	1.1	43
140	Fission of Entangled Spins: An Electronic Structure Perspective. Journal of Physical Chemistry Letters, 2013, 4, 3845-3852.	2.1	170
141	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.	2.0	14
142	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
143	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
144	Qâ€Chem: an engine for innovation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 317-326.	6.2	287

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145	Toward Organic Photohydrides: Excited-State Behavior of 10-Methyl-9-phenyl-9,10-dihydroacridine. Journal of Physical Chemistry B, 2013, 117, 15290-15296.	1.2	20
146	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. Journal of Physical Chemistry Letters, 2013, 4, 1743-1747.	2.1	25
147	On the Photodetachment from the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry A, 2013, 117, 11815-11822.	1.1	34
148	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
149	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
150	Overtone-induced dissociation and isomerization dynamics of the hydroxymethyl radical (CH2OH and) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	25
151	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, 12398-12405.	1.2	20
152	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
153	Electronic States of the Benzene Dimer: A Simple Case of Complexity. Journal of Physical Chemistry A, 2012, 116, 653-662.	1.1	43
154	Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of hydrogen bonds. Nature Chemistry, 2012, 4, 323-329.	6.6	69
155	De-perturbative corrections for charge-stabilized double ionization potential equation-of-motion coupled-cluster method. Journal of Chemical Physics, 2012, 136, 244109.	1.2	21
156	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
157	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
158	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
159	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
160	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
161	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
162	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, 1912-1920.	2.3	25

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163	The effect of microhydration on ionization energies of thymine. Faraday Discussions, 2011, 150, 313.	1.6	38
164	Spectroscopy and Fragmentation of Undercoordinated Bromoiridates. Journal of Physical Chemistry A, 2011, 115, 13482-13488.	1.1	0
165	What Drives the Redox Properties of Model Green Fluorescence Protein Chromophores?. Journal of Physical Chemistry Letters, 2011, 2, 2593-2597.	2.1	23
166	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
167	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
168	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
169	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
170	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
171	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
172	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
173	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
174	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
175	Frozen natural orbitals for ionized states within equation-of-motion coupled-cluster formalism. Journal of Chemical Physics, 2010, 132, 014109.	1.2	103
176	Spectroscopic signatures of proton transfer dynamics in the water dimer cation. Journal of Chemical Physics, 2010, 132, 194311.	1.2	69
177	The effect of oxidation on the electronic structure of the green fluorescent protein chromophore. Journal of Chemical Physics, 2010, 132, 115104.	1.2	32
178	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
179	Zooming into Ï€-Stacked Manifolds of Nucleobases: Ionized States of Dimethylated Uracil Dimers. Journal of Physical Chemistry A, 2010, 114, 2001-2009.	1.1	19
180	Electronic Structure and Spectroscopy of Oxyallyl: A Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 6935-6943.	1.1	28

#	Article	IF	Citations
181	Ionization-Induced Structural Changes in Uracil Dimers and Their Spectroscopic Signatures. Journal of Chemical Theory and Computation, 2010, 6, 705-717.	2.3	21
182	Roaming Pathway Leading to Unexpected Water + Vinyl Products in C₂H₄OH Dissociation. Journal of Physical Chemistry Letters, 2010, 1, 3058-3065.	2.1	62
183	Products of the Benzene + O(³P) Reaction. Journal of Physical Chemistry A, 2010, 114, 3355-3370.	1.1	92
184	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
185	Ionization of cytosine monomer and dimer studied by VUV photoionization and electronic structure calculations. Physical Chemistry Chemical Physics, 2010, 12, 2860.	1.3	65
186	Electronically excited and ionized states of the CH2CH2OH radical: A theoretical study. Journal of Chemical Physics, 2010, 132, 114308.	1.2	7
187	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
188	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
189	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
190	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
191	Preface to the Robert Benny Gerber Festschrift. Journal of Physical Chemistry A, 2009, 113, 7161-7162.	1.1	0
192	Multiphoton Ionization and Dissociation of Diazirine: A Theoretical and Experimental Study. Journal of Physical Chemistry A, 2009, 113, 7412-7421.	1.1	14
193	Ab Initio Calculation of the Photoelectron Spectra of the Hydroxycarbene Diradicals. Journal of Physical Chemistry A, 2009, 113, 7802-7809.	1.1	28
194	Effect of a Heteroatom on Bonding Patterns and Triradical Stabilization Energies of 2,4,6-Tridehydropyridine versus 1,3,5-Tridehydrobenzene. Journal of Physical Chemistry A, 2009, 113, 2591-2599.	1.1	21
195	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
196	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
197	Degree of Initial Hole Localization/Delocalization in Ionized Water Clusters. Journal of Physical Chemistry A, 2009, 113, 4423-4429.	1.1	35
198	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

#	Article	IF	Citations
199	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
200	Structure, vibrational frequencies, ionization energies, and photoelectron spectrum of the para-benzyne radical anion. Theoretical Chemistry Accounts, 2008, 120, 45-58.	0.5	24
201	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
202	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	1.1	115
203	Electronic Structure of the Water Dimer Cation. Journal of Physical Chemistry A, 2008, 112, 6159-6170.	1.1	84
204	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
205	Effect of Hyperconjugation on Ionization Energies of Hydroxyalkyl Radicals. Journal of Physical Chemistry A, 2008, 112, 9965-9969.	1.1	14
206	Conical for Stepwise, Glancing for Concerted: The Role of the Excited-State Topology in the Three-Body Dissociation of sym-Triazine. Journal of Physical Chemistry A, 2008, 112, 12345-12354.	1.1	18
207	The Role of Excited-State Topology in Three-Body Dissociation of sym -Triazine. Science, 2008, 321, 826-830.	6.0	38
208	Charge localization and Jahnâ€“Teller distortions in the benzene dimer cation. Journal of Chemical Physics, 2008, 129, 074104.	1.2	88
209	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
210	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
211	Electronic structure of the benzene dimer cation. Journal of Chemical Physics, 2007, 127, 044317.	1.2	61
212	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
213	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
214	Breaking the Curse of the Non-Dynamical Correlation Problem: The Spin-Flip Method. ACS Symposium Series, 2007, , 89-102.	0.5	11
215	Direct location of the minimum point on intersection seams of potential energy surfaces with equation-of-motion coupled-cluster methods. Molecular Physics, 2007, 105, 2515-2525.	0.8	20
216	Theoretical and Experimental Investigations of the Electronic Rydberg States of Diazomethane:â€‰ Assignments and State Interactions. Journal of Physical Chemistry A, 2007, 111, 4557-4566.	1.1	9

#	Article	IF	Citations
217	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
218	Vibronic Structure and Ion Core Interactions in Rydberg States of Diazomethane:â€‰ An Experimental and Theoretical Investigation. Journal of Physical Chemistry A, 2007, 111, 13347-13357.	1.1	3
219	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
220	Electronic Structure of Carbon Trioxide and Vibronic Interactions Involving Jahnâ˜Teller States. Journal of Physical Chemistry A, 2007, 111, 8271-8276.	1.1	28
221	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
222	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
223	Femtosecond Multidimensional Imaging of a Molecular Dissociation. Science, 2006, 311, 219-222.	6.0	164
224	Spectroscopy of the Cyano Radical in an Aqueous Environment. Journal of Physical Chemistry A, 2006, 110, 4854-4865.	1.1	21
225	Efficient Strategies for Accurate Calculations of Electronic Excitation and Ionization Energies:â€‰ Theory and Application to the Dehydro-m-xylylene Anion. Journal of Physical Chemistry A, 2006, 110, 291-298.	1.1	14
226	Beyond Vinyl:Â Electronic Structure of Unsaturated Propen-1-yl, Propen-2-yl, 1-Buten-2-yl, andtrans-2-Buten-2-yl Hydrocarbon Radicals. Journal of Physical Chemistry A, 2006, 110, 2746-2758.	1.1	20
227	Electronic structure of the two dehydro-meta-xylylene triradicals and their derivatives. Chemical Physics Letters, 2006, 425, 196-200.	1.2	11
228	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
229	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
230	Conical and glancing Jahn-Teller intersections in the cyclic trinitrogen cation. Journal of Chemical Physics, 2006, 124, 224309.	1.2	42
231	Spin-conserving and spin-flipping equation-of-motion coupled-cluster method with triple excitations. Journal of Chemical Physics, 2005, 123, 084107.	1.2	107
232	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
233	Triradicals. Journal of Physical Chemistry A, 2005, 109, 10638-10645.	1.1	87
234	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

#	Article	IF	Citations
235	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
236	Reactivity and Structure of the 5-Dehydro-m-xylylene Anion. Journal of Organic Chemistry, 2004, 69, 5735-5741.	1.7	16
237	Bonding Patterns in Benzene Triradicals from Structural, Spectroscopic, and Thermochemical Perspectives. Journal of Physical Chemistry A, 2004, 108, 6581-6588.	1.1	69
238	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
239	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
240	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
241	Rydbergâ€“valence interactions in CH2Clâ†’CH2+Cl photodissociation: Dependence of absorption probability on ground state vibrational excitation. Journal of Chemical Physics, 2003, 118, 9233-9240.	1.2	15
242	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
243	Electronic structure of the Ï€-bonded Alâ€“C2H4 complex: Characterization of the ground and low-lying excited states. Journal of Chemical Physics, 2003, 118, 10912-10918.	1.2	9
244	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
245	Electronic Structure of Halogen-Substituted Methyl Radicals:Â Equilibrium Geometries and Vibrational Spectra of CH2Cl and CH2F. Journal of Physical Chemistry A, 2002, 106, 5169-5176.	1.1	14
246	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
247	Singlet-triplet gaps in diradicals by the spin-flip approach: A benchmark study. Journal of Chemical Physics, 2002, 117, 4694-4708.	1.2	321
248	Size-consistent wave functions for bond-breaking: the equation-of-motion spin-flip model. Chemical Physics Letters, 2001, 338, 375-384.	1.2	430
249	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
250	Electronic structure of halogen-substituted methyl radicals: Excited states of CH2Cl and CH2F. Journal of Chemical Physics, 2001, 115, 7485-7494.	1.2	17
251	Small doped [sup 3]He clusters: A systematic quantum chemistry approach to fermionic nuclear wave functions and energies. Journal of Chemical Physics, 2001, 115, 10214.	1.2	23
252	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	1.5	617

#	Article	IF	Citations
253	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
254	Spin-contamination of coupled-cluster wave functions. Journal of Chemical Physics, 2000, 113, 6052-6062.	1.2	87
255	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
256	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
257	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
258	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
259	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
260	Photodissociation dynamics of HCl in solid Ar: Cage exit, nonadiabatic transitions, and recombination. Journal of Chemical Physics, 1997, 106, 6574-6587.	1.2	62
261	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
262	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
263	Nonadiabatic dynamics and electronic energy relaxation of Cl(2P) atoms in solid Ar. Journal of Chemical Physics, 1996, 105, 4626-4635.	1.2	54
264	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
265	Dissociative electron attachment in C2H via electronic resonances. Molecular Physics, 0, , .	0.8	2