Xiaosong Li

List of Publications by Citations

177 papers	5,837 citations	42 h-index	68 g-index
194 ext. papers	6,784 ext. citations	6.4 avg, IF	6.21 L-index

#	Paper	IF	Citations
177	Energy-Represented Direct Inversion in the Iterative Subspace within a Hybrid Geometry Optimization Method. *Journal of Chemical Theory and Computation*, **2006**, 2, 835-9	6.4	324
176	Ab initio Ehrenfest dynamics. *Journal of Chemical Physics*, **2005**, 123, 084106	3.9	269
175	Mixed Cation FAxPEA1−xPbI3 with Enhanced Phase and Ambient Stability toward High-Performance Perovskite Solar Cells. *Advanced Energy Materials*, **2017**, 7, 1601307	21.8	237
174	Doping of fullerenes via anion-induced electron transfer and its implication for surfactant facilitated high performance polymer solar cells. *Advanced Materials*, **2013**, 25, 4425-30	24	220
173	A time-dependent Hartree-Fock approach for studying the electronic optical response of molecules in intense fields. *Physical Chemistry Chemical Physics*, **2005**, 7, 233-9	3.6	159
172	Highly Efficient Organic Solar Cells Based on S,N-Heteroacene Non-Fullerene Acceptors. *Chemistry of Materials*, **2018**, 30, 5429-5434	9.6	158
171	Charge-controlled magnetism in colloidal doped semiconductor nanocrystals. *Nature Nanotechnology*, **2009**, 4, 681-7	28.7	135
170	Time-dependent density functional theory Ehrenfest dynamics: collisions between atomic oxygen and graphite clusters. *Journal of Chemical Physics*, **2007**, 126, 134307	3.9	120
169	Ab initio molecular dynamics studies of the photodissociation of formaldehyde, H2CO→H2+CO: Direct classical trajectory calculations by MP2 and density functional theory. *Journal of Chemical Physics*, **2000**, 113, 10062-10067	3.9	119
168	Single-Crystal and Electronic Structure of a 1.3 nm Indium Phosphide Nanocluster. *Journal of the American Chemical Society*, **2016**, 138, 1510-3	16.4	118
167	Solution-processible highly conducting fullerenes. *Advanced Materials*, **2013**, 25, 2457-61	24	113
166	Tailoring the Functionality of Organic Spacer Cations for Efficient and Stable Quasi-2D Perovskite Solar Cells. *Advanced Functional Materials*, **2019**, 29, 1900221	15.6	94
165	Real-time time-dependent electronic structure theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1341	7.9	89
164	Electronic optical response of molecules in intense fields: comparison of TD-HF, TD-CIS, and TD-CIS(D) approaches. *Journal of Chemical Physics*, **2007**, 126, 244110	3.9	84
163	Energy-Specific Linear Response TDHF/TDDFT for Calculating High-Energy Excited States. *Journal of Chemical Theory and Computation*, **2011**, 7, 3540-7	6.4	83
162	Interplay of Mobile Ions and Injected Carriers Creates Recombination Centers in Metal Halide Perovskites under Bias. *ACS Energy Letters*, **2018**, 3, 1279-1286	20.1	81
161	Modulation of Fluorescent Protein Chromophores To Detect Protein Aggregation with Turn-On Fluorescence. *Journal of the American Chemical Society*, **2018**, 140, 7381-7384	16.4	78

160	Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy. *Journal of Chemical Theory and Computation*, **2015**, 11, 4146-53	6.4	76
159	Mid-Gap States and Normal vs Inverted Bonding in Luminescent Cu- and Ag-Doped CdSe Nanocrystals. *Journal of the American Chemical Society*, **2017**, 139, 6411-6421	16.4	69
158	Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy. *Journal of the American Chemical Society*, **2016**, 138, 8752-64	16.4	67
157	Tunable Band Gap and Long Carrier Recombination Lifetime of Stable Mixed CH3NH3PbxSn1Br3 Single Crystals. *Chemistry of Materials*, **2018**, 30, 1556-1565	9.6	63
156	An efficient method for calculating dynamical hyperpolarizabilities using real-time time-dependent density functional theory. *Journal of Chemical Physics*, **2013**, 138, 064104	3.9	63
155	Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements. *Journal of Chemical Theory and Computation*, **2015**, 11, 2994-9	6.4	61
154	Long-Lived, Non-Geminate, Radiative Recombination of Photogenerated Charges in a Polymer/Small-Molecule Acceptor Photovoltaic Blend. *Journal of the American Chemical Society*, **2018**, 140, 9996-10008	16.4	61
153	Real-Time Time-Dependent Electronic Structure Theory. *Chemical Reviews*, **2020**, 120, 9951-9993	68.1	60
152	Efficient first-principles electronic dynamics. *Journal of Chemical Physics*, **2011**, 134, 184102	3.9	54
151	Investigation of pure and Co2+-doped ZnO quantum dot electronic structures using the density functional theory: choosing the right functional. *New Journal of Physics*, **2008**, 10, 055013	2.9	54
150	Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals: Oxidation States, JahnTeller Distortions, Vibronic Bandshapes, and SingletTriplet Splittings. *Journal of Physical Chemistry C*, **2016**, 120, 5714-5723	3.8	52
149	Density matrix search using direct inversion in the iterative subspace as a linear scaling alternative to diagonalization in electronic structure calculations. *Journal of Chemical Physics*, **2003**, 119, 7651-7658	3.9	51
148	Quantum coherent plasmon in silver nanowires: a real-time TDDFT study. *Journal of Chemical Physics*, **2014**, 140, 244705	3.9	50
147	Real time propagation of the exact two component time-dependent density functional theory. *Journal of Chemical Physics*, **2016**, 145, 104107	3.9	50
146	Structural Diversity in Cesium Bismuth Halide Nanocrystals. *Chemistry of Materials*, **2019**, 31, 4685-4697	9.6	49
145	Cation Exchange Induced Transformation of InP Magic-Sized Clusters. *Chemistry of Materials*, **2017**, 29, 7984-7992	9.6	49
144	Modeling the doubly excited state with time-dependent Hartree-Fock and density functional theories. *Journal of Chemical Physics*, **2008**, 129, 204107	3.9	49
143	Two-Component Noncollinear Time-Dependent Spin Density Functional Theory for Excited State Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 2591-2603	6.4	48

142	Ultrafast Coherent Electron-Hole Separation Dynamics in a Fullerene Derivative. *Journal of Physical Chemistry Letters*, **2011**, 2, 1189-92	6.4	48
141	Orbital pathways for Mn2+-carrier sp exchange in diluted magnetic semiconductor quantum dots. *Physical Review B*, **2011**, 84,	3.3	47
140	The Cation-Interaction Enables a Halo-Tag Fluorogenic Probe for Fast No-Wash Live Cell Imaging and Gel-Free Protein Quantification. *Biochemistry*, **2017**, 56, 1585-1595	3.2	45
139	Theoretical Characterization of Electronic Transitions in Co2+- and Mn2+-Doped ZnO Nanocrystals. *Journal of Physical Chemistry C*, **2009**, 113, 8710-8717	3.8	45
138	Investigating the role of amine in InP nanocrystal synthesis: destabilizing cluster intermediates by Z-type ligand displacement. *Chemical Communications*, **2016**, 53, 161-164	5.8	44
137	From charge-transfer to a charge-separated state: a perspective from the real-time TDDFT excitonic dynamics. *Physical Chemistry Chemical Physics*, **2014**, 16, 24457-65	3.6	44
136	Singlet-Triplet Transitions in Real-Time Time-Dependent Hartree-Fock/Density Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2415-9	6.4	43
135	Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures. *Journal of Chemical Theory and Computation*, **2016**, 12, 3711-8	6.4	41
134	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. *Journal of Physical Chemistry C*, **2015**, 119, 6421-6427	3.8	40
133	On the gauge invariance of nonperturbative electronic dynamics using the time-dependent Hartree-Fock and time-dependent Kohn-Sham. *Journal of Chemical Physics*, **2011**, 135, 164101	3.9	40
132	Surface hopping with Ehrenfest excited potential. *Journal of Chemical Physics*, **2011**, 135, 144102	3.9	40
131	"Watching" Polaron Pair Formation from First-Principles Electron-Nuclear Dynamics. *Journal of Physical Chemistry A*, **2016**, 120, 7255-61	2.8	39
130	An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables. *European Physical Journal B*, **2018**, 91, 1	1.2	35
129	Direct ab Initio (Meta-)Surface-Hopping Dynamics. *Journal of Chemical Theory and Computation*, **2016**, 12, 935-45	6.4	34
128	Ab initio time-resolved density functional theory for lifetimes of excited adsorbate states at metal surfaces. *Chemical Physics Letters*, **2007**, 439, 199-203	2.5	33
127	Glyoxal photodissociation. An ab initio direct classical trajectory study of C2H2O2-H2+2 CO. *Journal of Chemical Physics*, **2001**, 114, 8897-8904	3.9	33
126	Ehrenfest dynamics with a time-dependent density-functional-theory calculation of lifetimes and resonant widths of charge-transfer states of Li+ near an aluminum cluster surface. *Physical Review A*, **2009**, 80,	2.6	32
125	An atomic orbital based real-time time-dependent density functional theory for computing electronic circular dichroism band spectra. *Journal of Chemical Physics*, **2016**, 144, 234102	3.9	32

124	Solvated First-Principles Excited-State Charge-Transfer Dynamics with Time-Dependent Polarizable Continuum Model and Solvent Dielectric Relaxation. *Journal of Physical Chemistry Letters*, **2012**, 3, 2898-2904	6.4	31
123	AggFluor: Fluorogenic Toolbox Enables Direct Visualization of the Multi-Step Protein Aggregation Process in Live Cells. *Journal of the American Chemical Society*, **2020**, 142, 17515-17523	16.4	31
122	The Chronus Quantum software package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1436	7.9	31
121	Modeling L-Edge X-ray Absorption Spectroscopy with Real-Time Exact Two-Component Relativistic Time-Dependent Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 1998-2006	5.4	30
120	Ab Initio Transient Vibrational Spectral Analysis. *Journal of Physical Chemistry Letters*, **2016**, 7, 4501-4508	6.4	30
119	Theoretical Characterization of Conduction-Band Electrons in Photodoped and Aluminum-Doped Zinc Oxide (AZO) Quantum Dots. *Journal of Physical Chemistry C*, **2014**, 118, 26584-26590	3.8	29
118	Assessment of low-scaling approximations to the equation of motion coupled-cluster singles and doubles equations. *Journal of Chemical Physics*, **2014**, 141, 164116	3.9	29
117	Time-dependent density functional theory calculations of Ehrenfest dynamics of laser controlled dissociation of NO+: pulse length and sequential multiple single-photon processes. *Journal of Physical Chemistry A*, **2010**, 114, 6201-6	2.8	29
116	A numerical simulation of nonadiabatic electron excitation in the strong field regime: Linear polyenes. *Journal of Physical Chemistry A*, **2005**, 109, 5176-85	2.8	29
115	Doping Versatile n-Type Organic Semiconductors via Room Temperature Solution-Processable Anionic Dopants. *ACS Applied Materials & Interfaces*, **2017**, 9, 1136-1144	9.5	28
114	Time-dependent non-equilibrium dielectric response in QM/continuum approaches. *Journal of Chemical Physics*, **2015**, 142, 034120	3.9	28
113	Realization of a Highly Oriented MAPbBr3 Perovskite Thin Film via Ion Exchange for Ultrahigh Color Purity Green Light Emission. *ACS Energy Letters*, **2018**, 3, 1662-1669	20.1	28
112	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. *Journal of Chemical Physics*, **2015**, 143, 234103	3.9	28
111	Ferromagnetic excited-state Mn2+ dimers in Zn1−xMnxSe quantum dots observed by time-resolved magnetophotoluminescence. *Physical Review B*, **2014**, 89,	3.3	28
110	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. *Physical Review B*, **2016**, 94,	3.3	28
109	Real-Time Time-Dependent Nuclear-Electronic Orbital Approach: Dynamics beyond the Born-Oppenheimer Approximation. *Journal of Physical Chemistry Letters*, **2020**, 11, 4052-4058	6.4	27
108	High-pressure, high-temperature molecular doping of nanodiamond. *Science Advances*, **2019**, 5, eaau6073	14.3	25
107	Stability of the complex generalized Hartree-Fock equations. *Journal of Chemical Physics*, **2015**, 142, 154109	3.9	25

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105	Modeling ultrafast solvated electronic dynamics using time-dependent density functional theory and polarizable continuum model. *Journal of Physical Chemistry A*, **2012**, 116, 1884-90	2.8	25
104	Numerical simulation of nonadiabatic electron excitation in the strong field regime. 2. Linear polyene cations. *Journal of Physical Chemistry A*, **2005**, 109, 10527-34	2.8	25
103	Soluble Supercapacitors: Large and Reversible Charge Storage in Colloidal Iron-Doped ZnO Nanocrystals. *Nano Letters*, **2018**, 18, 3297-3302	11.5	24
102	Generalized Hartree-Fock with Nonperturbative Treatment of Strong Magnetic Fields: Application to Molecular Spin Phase Transitions. *Journal of Chemical Theory and Computation*, **2019**, 15, 348-356	6.4	22
101	Non-adiabatic molecular dynamics investigation of photoionization state formation and lifetime in Mn^{2+}-doped ZnO quantum dots. *Physical Chemistry Chemical Physics*, **2014**, 16, 17507-14	3.6	21
100	Solvent effects on intramolecular charge transfer dynamics in a fullerene derivative. *Journal of Physical Chemistry A*, **2013**, 117, 2687-91	2.8	21
99	Modeling L-edge X-ray absorption spectroscopy with linear response exact two-component relativistic time-dependent density functional theory. *Journal of Chemical Physics*, **2019**, 150, 234103	3.9	20
98	A Guided Self-Consistent-Field Method for Excited-State Wave Function Optimization: Applications to Ligand-Field Transitions in Transition-Metal Complexes. *Journal of Chemical Theory and Computation*, **2013**, 9, 3933-8	6.4	20
97	Molecular Vibration Induced Plasmon Decay. *Journal of Physical Chemistry C*, **2017**, 121, 15368-15374	3.8	20
96	Numerical simulation of nonadiabatic electron excitation in the strong-field regime. 3. Polyacene neutrals and cations. *Journal of Physical Chemistry A*, **2007**, 111, 6920-32	2.8	20
95	A Hybrid Quantum-Classical Model of Electrostatics in Multiply Charged Quantum Dots. *Journal of Physical Chemistry C*, **2017**, 121, 26086-26095	3.8	19
94	Effect of Surface Passivation on Nanodiamond Crystallinity. *Journal of Physical Chemistry C*, **2018**, 122, 8573-8580	3.8	19
93	Current development of noncollinear electronic structure theory. *International Journal of Quantum Chemistry*, **2018**, 118, e25398	2.1	19
92	Ab initio non-relativistic spin dynamics. *Journal of Chemical Physics*, **2014**, 141, 214111	3.9	19
91	Ferromagnetism in p-Type Manganese-Doped Zinc Oxide Quantum Dots. *Journal of Physical Chemistry Letters*, **2012**, 3, 1374-80	6.4	19
90	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. *Journal of Chemical Theory and Computation*, **2017**, 13, 2789-2803	6.4	18
89	Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. *Journal of Physical Chemistry Letters*, **2017**, 8, 5283-5289	6.4	18

88	Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires. *Journal of Physical Chemistry C*, **2019**, 123, 14734-14745	3.8	18
87	Effect of Excited-State Structural Relaxation on Midgap Excitations in Co2+-Doped ZnO Quantum Dots. *Journal of Physical Chemistry C*, **2014**, 118, 13152-13156	3.8	18
86	Excited-State Double Exchange in Manganese-Doped ZnO Quantum Dots: A Time-Dependent Density-Functional Study. *Journal of Physical Chemistry Letters*, **2010**, 1, 1927-1931	6.4	18
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84	An ab Initio Linear Response Method for Computing Magnetic Circular Dichroism Spectra with Nonperturbative Treatment of Magnetic Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 3162-3169	6.4	17
83	Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory. *Journal of the American Chemical Society*, **2015**, 137, 14743-50	16.4	17
82	Mechanisms of bridge-mediated electron transfer: a TDDFT electronic dynamics study. *Journal of Chemical Physics*, **2012**, 137, 22A512	3.9	17
81	Mapping Vibronic Couplings in a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronic-Vibrational Spectroscopy. *Journal of Physical Chemistry Letters*, **2018**, 9, 6289-6295	6.4	17
80	Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters. *Journal of Physical Chemistry Letters*, **2019**, 10, 1833-1839	6.4	16
79	Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster. *Journal of Chemical Theory and Computation*, **2019**, 15, 6617-6624	6.4	16
78	Characterization of Excited-State Magnetic Exchange in Mn2+-Doped ZnO Quantum Dots Using Time-Dependent Density Functional Theory. *Journal of Physical Chemistry C*, **2011**, 115, 20986-20991	3.8	15
77	Laser-controlled dissociation of C2H2(2+): Ehrenfest dynamics using time-dependent density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 3463-9	2.8	15
76	Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 43-51	6.4	15
75	A conductive liquid crystal via facile doping of an n-type benzodifurandione derivative. *Journal of Materials Chemistry A*, **2015**, 3, 6929-6934	13	14
74	Time-Dependent Configuration Interaction Using the Graphical Unitary Group Approach: Nonlinear Electric Properties. *Advances in Quantum Chemistry*, **2018**, 76, 295-313	1.4	14
73	Ab Initio Excited-State Transient Raman Analysis. *Journal of Physical Chemistry A*, **2017**, 121, 3958-3965	2.8	13
72	Resolving the ultrafast intersystem crossing in a bimetallic platinum complex. *Journal of Chemical Physics*, **2019**, 151, 114303	3.9	13
71	Nuclear-electronic orbital Ehrenfest dynamics. *Journal of Chemical Physics*, **2020**, 153, 224111	3.9	13

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68	Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2019**, 15, 1633-1641	6.4	12
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66	Anisotropic Polarizability-Induced Plasmon Transfer. *Journal of Physical Chemistry C*, **2018**, 122, 10621-10626	3.8	12
65	Accelerating Real-Time Time-Dependent Density Functional Theory with a Nonrecursive Chebyshev Expansion of the Quantum Propagator. *Journal of Chemical Theory and Computation*, **2016**, 12, 5333-5338	6.4	12
64	Relativistic Two-Component Particle-Particle Tamm-Dancoff Approximation. *Journal of Chemical Theory and Computation*, **2016**, 12, 5379-5384	6.4	12
63	Orientation-dependent imaging of electronically excited quantum dots. *Journal of Chemical Physics*, **2018**, 148, 064701	3.9	11
62	Efficient Implementation of Variation after Projection Generalized Hartree-Fock. *Journal of Chemical Theory and Computation*, **2018**, 14, 588-596	6.4	11
61	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. *Chirality*, **2018**, 30, 850-865	2.1	11
60	A Well-Tempered Hybrid Method for Solving Challenging Time-Dependent Density Functional Theory (TDDFT) Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 2034-2041	6.4	11
59	Classical or Quantum? A Computational Study of Small Ion Diffusion in II-VI Semiconductor Quantum Dots. *Journal of Physical Chemistry C*, **2016**, 120, 19434-19441	3.8	11
58	Simulating Magnetic Circular Dichroism Spectra with Real-Time Time-Dependent Density Functional Theory in Gauge Including Atomic Orbitals. *Journal of Chemical Theory and Computation*, **2019**, 15, 6824-6831	6.4	11
57	Effects of Crystallographic and Shape Anisotropies on Dopant-Carrier Exchange Interactions in Magnetic Semiconductor Quantum Dots. *Journal of Physical Chemistry C*, **2014**, 118, 7630-7636	3.8	11
56	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. *Journal of Chemical Theory and Computation*, **2017**, 13, 4950-4961	6.4	11
55	Open-system electronic dynamics and thermalized electronic structure. *Journal of Chemical Physics*, **2011**, 134, 024118	3.9	11
54	Frequency and Time Domain Nuclear-Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronic-Protonic Double Excitations. *Journal of Physical Chemistry Letters*, **2020**, 11, 6435-6442	6.4	11
53	Natural transition orbitals for complex two-component excited state calculations. *Journal of Computational Chemistry*, **2020**, 41, 1557-1563	3.5	10

52	Relativistic Two-Component Multireference Configuration Interaction Method with Tunable Correlation Space. *Journal of Chemical Theory and Computation*, **2020**, 16, 2975-2984	6.4	10
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50	Exciton Coherence Length and Dynamics in Graphene Quantum Dot Assemblies. *Journal of Physical Chemistry Letters*, **2020**, 11, 210-216	6.4	10
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45	Electronic structures and spectroscopic signatures of silicon-vacancy containing nanodiamonds. *Physical Review B*, **2018**, 98,	3.3	9
44	Toward the evaluation of intersystem crossing rates with variational relativistic methods. *Journal of Chemical Physics*, **2019**, 151, 084107	3.9	8
43	Role of Vibrational Dynamics on Excited-State Electronic Coherence in a Binuclear Platinum Complex. *Journal of Physical Chemistry A*, **2018**, 122, 5071-5077	2.8	8
42	Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. *Journal of Chemical Theory and Computation*, **2021**, 17, 277-289	6.4	8
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40	Relationship between Hydrogen-Bonding Motifs and the 1b Splitting in the X-ray Emission Spectrum of Liquid Water. *Journal of Physical Chemistry Letters*, **2021**, 12, 3996-4002	6.4	8
39	Modeling Magneto-Photoabsorption Using Time-Dependent Complex Generalized Hartree-Fock. *ChemPhotoChem*, **2019**, 3, 739-746	3.3	7
38	X-ray absorption signatures of hydrogen-bond structure in water□alcohol solutions. *International Journal of Quantum Chemistry*, **2019**, 119, e25802	2.1	7
37	Iron-Content-Dependent, Quasi-Static Dielectric Resonances and Oxidative Transitions in Bornite and Chalcopyrite Copper Iron Sulfide Nanocrystals. *Chemistry of Materials*, **2021**, 33, 1821-1831	9.6	7
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35	Relativistic Effects in Magnetic Circular Dichroism: Restricted Magnetic Balance and Temperature Dependence. *Journal of Chemical Theory and Computation*, **2020**, 16, 4533-4542	6.4	6

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33	Embedding non-collinear two-component electronic structure in a collinear quantum environment. *Journal of Chemical Physics*, **2019**, 150, 174114	3.9	4
32	Unveiling ultrafast dynamics in bridged bimetallic complexes using optical and X-ray transient absorption spectroscopies.. *Chemical Science*, **2022**, 13, 1715-1724	9.4	4
31	Photophysics of graphene quantum dot assemblies with axially coordinated cobaloxime catalysts. *Journal of Chemical Physics*, **2020**, 153, 124903	3.9	4
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29	Efficient Four-Component Dirac-Coulomb-Gaunt Hartree-Fock in the Pauli Spinor Representation. *Journal of Chemical Theory and Computation*, **2021**, 17, 3388-3402	6.4	4
28	Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?. *Journal of Physical Chemistry Letters*, **2016**, 7, 5193-5197	6.4	4
27	Defect-Induced Magnetic Skyrmion in a Two-Dimensional Chromium Triiodide Monolayer. *Jacs Au*, **2021**, 1, 1362-1367		4
26	Tunable Band-Edge Potentials and Charge Storage in Colloidal Tin-Doped Indium Oxide (ITO) Nanocrystals. *ACS Nano*, **2021**, 15, 14116-14124	16.7	4
25	Theoretical investigation of quantum confinement on the Rashba effect in ZnO semiconductor nanocrystals. *Journal of Chemical Physics*, **2020**, 152, 014308	3.9	3
24	Relativistic two-component projection-based quantum embedding for open-shell systems. *Journal of Chemical Physics*, **2020**, 153, 094113	3.9	3
23	The "Hole" Story in Ionized Water from the Perspective of Ehrenfest Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 9946-9951	6.4	3
22	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. *Journal of Physical Chemistry A*, **2020**, 124, 9729-9737	2.8	3
21	Interplays of electron and nuclear motions along CO dissociation trajectory in myoglobin revealed by ultrafast X-rays and quantum dynamics calculations. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
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19	Tuning the interfacial stoichiometry of InP core and InP/ZnSe core/shell quantum dots. *Journal of Chemical Physics*, **2021**, 155, 084701	3.9	3
18	General Design Rules for Bimetallic Platinum(II) Complexes. *Journal of Physical Chemistry A*, **2021**, 125, 9438-9449	2.8	2
17	Determination of the SmO bond energy by threshold photodissociation of the cryogenically cooled ion. *Journal of Chemical Physics*, **2021**, 155, 174303	3.9	2

List of Publications

16	Spectroscopic Signatures of the B and H4 Polyatomic Nitrogen Aggregates in Nanodiamond. *Journal of Physical Chemistry C*, **2020**, 124, 18275-18283	3.8	2
15	Perspective on Kramers symmetry breaking and restoration in relativistic electronic structure methods for open-shell systems. *Journal of Chemical Physics*, **2020**, 153, 090903	3.9	2
14	Localized relativistic two-component methods for ground and excited state calculations. *Annual Reports in Computational Chemistry*, **2020**, 16, 17-37	1.8	2
13	Short Iterative Lanczos Integration in Time-Dependent Equation-of-Motion Coupled-Cluster Theory. *Journal of Physical Chemistry A*, **2021**, 125, 5438-5447	2.8	2
12	Intersystem Crossings in Late-Row Elements: A Perspective.. *Journal of Physical Chemistry Letters*, **2022**, 3039-3046	6.4	2
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