Xiaosong Li

List of Publications by Year in descending order

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		50170	66788
189	7,767	46	78
papers	citations	h-index	g-index

194	194	194	7985
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Bimetallic Copper/Ruthenium/Osmium Complexes: Observation of Conformational Differences Between the Solution Phase and Solid State by Atomic Pair Distribution Function Analysis. Angewandte Chemie - International Edition, 2022, 61, e202111764.	7.2	5
2	Long-Lived Excited State in a Solubilized Graphene Nanoribbon. Journal of Physical Chemistry C, 2022, 126, 1946-1957.	1.5	1
3	Unveiling ultrafast dynamics in bridged bimetallic complexes using optical and X-ray transient absorption spectroscopies. Chemical Science, 2022, 13, 1715-1724.	3.7	14
4	Solvated Nuclearâ€“Electronic Orbital Structure and Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 1340-1346.	2.3	9
5	Relativistic Effects in Modeling the Ligand K-Edge X-ray Absorption Near-Edge Structure of Uranium Complexes. Journal of Chemical Theory and Computation, 2022, , .	2.3	3
6	Intersystem Crossings in Late-Row Elements: A Perspective. Journal of Physical Chemistry Letters, 2022, 13, 3039-3046.	2.1	11
7	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2947-2954.	2.3	7
8	Titelbild: Bimetallic Copper/Ruthenium/Osmium Complexes: Observation of Conformational Differences Between the Solution Phase and Solid State by Atomic Pair Distribution Function Analysis (Angew. Chem. 5/2022). Angewandte Chemie, 2022, 134, .	1.6	0
9	Phaseâ€Controlled Synthesis and Quasiâ€Static Dielectric Resonances in Silver Iron Sulfide (AgFeS) Tj ETQq1 1 0.784314 rgBT /Overl	5.2	2
10	Two-Component Multireference Restricted Active Space Configuration Interaction for the Computation of L-Edge X-ray Absorption Spectra. Journal of Chemical Theory and Computation, 2022, 18, 141-150.	2.3	9
11	Relativistic nonorthogonal configuration interaction: application to L_{2,3}-edge X-ray spectroscopy. Physical Chemistry Chemical Physics, 2022, 24, 10745-10756.	1.3	4
12	Exact-Two-Component Relativistic Multireference Second-Order Perturbation Theory. Journal of Chemical Theory and Computation, 2022, 18, 2983-2992.	2.3	11
13	Exploring Potential Energy Surfaces Using Reinforcement Machine Learning. Journal of Chemical Information and Modeling, 2022, 62, 3169-3179.	2.5	6
14	Proton-Coupled Electron Transfer in a Ruthenium(II) Bipyrimidine Complex in Its Ground and Excited Electronic States. Journal of Physical Chemistry A, 2022, 126, 4349-4358.	1.1	1
15	Efficient evaluation of the Breit operator in the Pauli spinor basis. Journal of Chemical Physics, 2022, 157, .	1.2	14
16	Highâ€Efficiency Quasiâ€2D Perovskite Solar Cells Incorporating 2,2â€²â€Biimidazolium Cation. Solar Rrl, 2021, 5, 2000700.	3.1	9
17	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.	3.2	17
18	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, .	3.3	10

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19	Relationship between Hydrogen-Bonding Motifs and the 1b₁ Splitting in the X-ray Emission Spectrum of Liquid Water. Journal of Physical Chemistry Letters, 2021, 12, 3996-4002.	2.1	21
20	Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 3497-3502.	2.1	31
21	Toward the Minimal Floating Operation Count Cholesky Decomposition of Electron Repulsion Integrals. Journal of Physical Chemistry A, 2021, 125, 4258-4265.	1.1	11
22	Efficient Four-Component Diracâ€“Coulombâ€“Gaunt Hartreeâ€“Fock in the Pauli Spinor Representation. Journal of Chemical Theory and Computation, 2021, 17, 3388-3402.	2.3	24
23	Short Iterative Lanczos Integration in Time-Dependent Equation-of-Motion Coupled-Cluster Theory. Journal of Physical Chemistry A, 2021, 125, 5438-5447.	1.1	12
24	Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic Î”SCF. Journal of Chemical Physics, 2021, 155, 014103.	1.2	5
25	Ultrafast Excited-State Dynamics of Photoluminescent Pt(II) Dimers Probed by a Coherent Vibrational Wavepacket. Journal of Physical Chemistry Letters, 2021, 12, 6794-6803.	2.1	23
26	Defect-Induced Magnetic Skyrmion in a Two-Dimensional Chromium Triiodide Monolayer. Jacs Au, 2021, 1, 1362-1367.	3.6	10
27	Tuning the interfacial stoichiometry of InP core and InP/ZnSe core/shell quantum dots. Journal of Chemical Physics, 2021, 155, 084701.	1.2	9
28	Reinforcement Learning Configuration Interaction. Journal of Chemical Theory and Computation, 2021, 17, 5482-5491.	2.3	9
29	Tunable Band-Edge Potentials and Charge Storage in Colloidal Tin-Doped Indium Oxide (ITO) Nanocrystals. ACS Nano, 2021, 15, 14116-14124.	7.3	8
30	Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. Journal of Chemical Theory and Computation, 2021, 17, 277-289.	2.3	18
31	General Design Rules for Bimetallic Platinum(II) Complexes. Journal of Physical Chemistry A, 2021, 125, 9438-9449.	1.1	7
32	Determination of the SmO+ bond energy by threshold photodissociation of the cryogenically cooled ion. Journal of Chemical Physics, 2021, 155, 174303.	1.2	15
33	Spin photovoltaic effect in magnetic van der Waals heterostructures. Science Advances, 2021, 7, eabg8094.	4.7	15
34	The Chronus Quantum software package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1436.	6.2	66
35	Theoretical investigation of quantum confinement on the Rashba effect in ZnO semiconductor nanocrystals. Journal of Chemical Physics, 2020, 152, 014308.	1.2	8
36	Exciton Coherence Length and Dynamics in Graphene Quantum Dot Assemblies. Journal of Physical Chemistry Letters, 2020, 11, 210-216.	2.1	14

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37	Photophysics of graphene quantum dot assemblies with axially coordinated cobaloxime catalysts. Journal of Chemical Physics, 2020, 153, 124903.	1.2	5
38	Relativistic two-component projection-based quantum embedding for open-shell systems. Journal of Chemical Physics, 2020, 153, 094113.	1.2	10
39	Spectroscopic Signatures of the B and H₄ Polyatomic Nitrogen Aggregates in Nanodiamond. Journal of Physical Chemistry C, 2020, 124, 18275-18283.	1.5	5
40	Frequency and Time Domain Nuclearâ€“Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronicâ€“Protonic Double Excitations. Journal of Physical Chemistry Letters, 2020, 11, 6435-6442.	2.1	15
41	The â€œHoleâ€•Story in Ionized Water from the Perspective of Ehrenfest Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 9946-9951.	2.1	8
42	Ultrafast Nonradiative Decay of a Dipolar Plasmon-like State in Naphthalene. Journal of Physical Chemistry A, 2020, 124, 9729-9737.	1.1	4
43	Efficient Intermolecular Energy Exchange and Soft Ionization of Water at Nanoplatelet Interfaces. Journal of Physical Chemistry Letters, 2020, 11, 10088-10093.	2.1	4
44	Electronic Structure and Nonadiabatic Dynamics of Atomic Silver Nanowireâ€“N₂ Systems. Journal of Physical Chemistry C, 2020, 124, 20834-20845.	1.5	15
45	Ultrafast Nonlinear Plasmon Decay Processes in Silver Nanoclusters. Journal of Physical Chemistry C, 2020, 124, 20477-20487.	1.5	9
46	Perspective on Kramers symmetry breaking and restoration in relativistic electronic structure methods for open-shell systems. Journal of Chemical Physics, 2020, 153, 090903.	1.2	7
47	Localized relativistic two-component methods for ground and excited state calculations. Annual Reports in Computational Chemistry, 2020, 16, 17-37.	0.9	6
48	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.	6.6	90
49	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	23.0	141
50	Natural transition orbitals for complex <scp>twoâ€component</scp> excited state calculations. Journal of Computational Chemistry, 2020, 41, 1557-1563.	1.5	15
51	Relativistic Two-Component Multireference Configuration Interaction Method with Tunable Correlation Space. Journal of Chemical Theory and Computation, 2020, 16, 2975-2984.	2.3	30
52	Real-Time Time-Dependent Nuclearâ€Electronic Orbital Approach: Dynamics beyond the Bornâ€“Oppenheimer Approximation. Journal of Physical Chemistry Letters, 2020, 11, 4052-4058.	2.1	48
53	Relativistic Effects in Magnetic Circular Dichroism: Restricted Magnetic Balance and Temperature Dependence. Journal of Chemical Theory and Computation, 2020, 16, 4533-4542.	2.3	13
54	Ab initio methods for L-edge x-ray absorption spectroscopy. Chemical Physics Reviews, 2020, 1, .	2.6	25

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55	Nuclearâ€“electronic orbital Ehrenfest dynamics. Journal of Chemical Physics, 2020, 153, 224111.	1.2	28
56	Embedding non-collinear two-component electronic structure in a collinear quantum environment. Journal of Chemical Physics, 2019, 150, 174114.	1.2	9
57	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.	2.3	19
58	Relativistic Real-Time Time-Dependent Equation-of-Motion Coupled-Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6617-6624.	2.3	40
59	Toward the evaluation of intersystem crossing rates with variational relativistic methods. Journal of Chemical Physics, 2019, 151, 084107.	1.2	11
60	Resolving the ultrafast intersystem crossing in a bimetallic platinum complex. Journal of Chemical Physics, 2019, 151, 114303.	1.2	19
61	Time-Dependent Complete Active Space Embedded in a Polarizable Force Field. Journal of Chemical Theory and Computation, 2019, 15, 1633-1641.	2.3	16
62	Structural Diversity in Cesium Bismuth Halide Nanocrystals. Chemistry of Materials, 2019, 31, 4685-4697.	3.2	80
63	Modeling L2,3-edge X-ray absorption spectroscopy with linear response exact two-component relativistic time-dependent density functional theory. Journal of Chemical Physics, 2019, 150, 234103.	1.2	28
64	Modeling Magnetoâ€Photoabsorption Using Timeâ€Dependent Complex Generalized Hartreeâ€Fock. ChemPhotoChem, 2019, 3, 739-746.	1.5	11
65	Real-Time TDDFT Investigation of Optical Absorption in Gold Nanowires. Journal of Physical Chemistry C, 2019, 123, 14734-14745.	1.5	31
66	The Role of Excited-State Proton Relays in the Photochemical Dynamics of Water Nanodroplets. Journal of Physical Chemistry Letters, 2019, 10, 3694-3698.	2.1	6
67	Tailoring the Functionality of Organic Spacer Cations for Efficient and Stable Quasiâ€2D Perovskite Solar Cells. Advanced Functional Materials, 2019, 29, 1900221.	7.8	144
68	High-pressure, high-temperature molecular doping of nanodiamond. Science Advances, 2019, 5, eaau6073.	4.7	40
69	Variational Relativistic Two-Component Complete-Active-Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2019, 15, 2974-2982.	2.3	28
70	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.	2.3	27
71	Carboxylate Anchors Act as Exciton Reporters in 1.3 nm Indium Phosphide Nanoclusters. Journal of Physical Chemistry Letters, 2019, 10, 1833-1839.	2.1	23
72	Nonequilibrium Environment Dynamics in a Frequency-Dependent Polarizable Embedding Model. Journal of Chemical Theory and Computation, 2019, 15, 43-51.	2.3	24

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73	Generalized Hartreeâ€“Fock with Nonperturbative Treatment of Strong Magnetic Fields: Application to Molecular Spin Phase Transitions. Journal of Chemical Theory and Computation, 2019, 15, 348-356.	2.3	33
74	Xâ€ray absorption signatures of hydrogenâ€bond structure in waterâ€“alcohol solutions. International Journal of Quantum Chemistry, 2019, 119, e25802.	1.0	13
75	Anticorrelated Contributions to Pre-edge Features of Aluminate Near-Edge X-ray Absorption Spectroscopy in Concentrated Electrolytes. Journal of Physical Chemistry Letters, 2018, 9, 2444-2449.	2.1	9
76	Soluble Supercapacitors: Large and Reversible Charge Storage in Colloidal Iron-Doped ZnO Nanocrystals. Nano Letters, 2018, 18, 3297-3302.	4.5	40
77	Effect of Surface Passivation on Nanodiamond Crystallinity. Journal of Physical Chemistry C, 2018, 122, 8573-8580.	1.5	24
78	Role of Vibrational Dynamics on Excited-State Electronic Coherence in a Binuclear Platinum Complex. Journal of Physical Chemistry A, 2018, 122, 5071-5077.	1.1	10
79	Tunable Band Gap and Long Carrier Recombination Lifetime of Stable Mixed CH₃NH₃Pb_xSn_{1â€“x}Br₃ Single Crystals. Chemistry of Materials, 2018, 30, 1556-1565.	3.2	93
80	Orientation-dependent imaging of electronically excited quantum dots. Journal of Chemical Physics, 2018, 148, 064701.	1.2	13
81	Efficient Implementation of Variation after Projection Generalized Hartreeâ€“Fock. Journal of Chemical Theory and Computation, 2018, 14, 588-596.	2.3	14
82	Computational simulation of vibrationally resolved spectra for spinâ€forbidden transitions. Chirality, 2018, 30, 850-865.	1.3	15
83	Anisotropic Polarizability-Induced Plasmon Transfer. Journal of Physical Chemistry C, 2018, 122, 10621-10626.	1.5	22
84	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.	2.3	15
85	Modeling L_{2,3}-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.	2.3	44
86	Current development of noncollinear electronic structure theory. International Journal of Quantum Chemistry, 2018, 118, e25398.	1.0	22
87	Realâ€time timeâ€dependent electronic structure theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1341.	6.2	122
88	Inverted solvatochromic Stokes shift in GFP-like chromophores with extended conjugation. Chinese Journal of Chemical Physics, 2018, 31, 599-607.	0.6	0
89	Electronic structures and spectroscopic signatures of silicon-vacancy containing nanodiamonds. Physical Review B, 2018, 98, .	1.1	16
90	Mapping Vibronic Couplings in a Solar Cell Dye with Polarization-Selective Two-Dimensional Electronicâ€“Vibrational Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 6289-6295.	2.1	31

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91	Time-Dependent Configuration Interaction Using the Graphical Unitary Group Approach: Nonlinear Electric Properties. Advances in Quantum Chemistry, 2018, 76, 295-313.	0.4	19
92	Highly Efficient Organic Solar Cells Based on S,N-Heteroacene Non-Fullerene Acceptors. Chemistry of Materials, 2018, 30, 5429-5434.	3.2	194
93	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.	6.6	73
94	An efficient implementation of two-component relativistic density functional theory with torque-free auxiliary variables. European Physical Journal B, 2018, 91, 1.	0.6	54
95	Interplay of Mobile Ions and Injected Carriers Creates Recombination Centers in Metal Halide Perovskites under Bias. ACS Energy Letters, 2018, 3, 1279-1286.	8.8	106
96	Modulation of Fluorescent Protein Chromophores To Detect Protein Aggregation with Turn-On Fluorescence. Journal of the American Chemical Society, 2018, 140, 7381-7384.	6.6	147
97	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.	8.8	38
98	The Cationâ^'Ï€ Interaction Enables a Halo-Tag Fluorogenic Probe for Fast No-Wash Live Cell Imaging and Gel-Free Protein Quantification. Biochemistry, 2017, 56, 1585-1595.	1.2	66
99	Can Excited State Electronic Coherence Be Tuned via Molecular Structural Modification? A First-Principles Quantum Electronic Dynamics Study of Pyrazolate-Bridged Pt(II) Dimers. Journal of Physical Chemistry A, 2017, 121, 1932-1939.	1.1	15
100	Mid-Gap States and Normal vs Inverted Bonding in Luminescent Cu⁺-Âand Ag⁺-Doped CdSe Nanocrystals. Journal of the American Chemical Society, 2017, 139, 6411-6421.	6.6	88
101	Ab Initio Excited-State Transient Raman Analysis. Journal of Physical Chemistry A, 2017, 121, 3958-3965.	1.1	16
102	Two-Component Noncollinear Time-Dependent Spin Density Functional Theory for Excited State Calculations. Journal of Chemical Theory and Computation, 2017, 13, 2591-2603.	2.3	66
103	Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route. Journal of Chemical Theory and Computation, 2017, 13, 2789-2803.	2.3	23
104	Investigating the role of amine in InP nanocrystal synthesis: destabilizing cluster intermediates by Z-type ligand displacement. Chemical Communications, 2017, 53, 161-164.	2.2	55
105	Doping Versatile n-Type Organic Semiconductors via Room Temperature Solution-Processable Anionic Dopants. ACS Applied Materials & Interfaces, 2017, 9, 1136-1144.	4.0	35
106	Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. Journal of Physical Chemistry Letters, 2017, 8, 5283-5289.	2.1	25
107	A Hybrid Quantum-Classical Model of Electrostatics in Multiply Charged Quantum Dots. Journal of Physical Chemistry C, 2017, 121, 26086-26095.	1.5	22
108	Cation Exchange Induced Transformation of InP Magic-Sized Clusters. Chemistry of Materials, 2017, 29, 7984-7992.	3.2	67

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109	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 4950-4961.	2.3	14
110	Molecular Vibration Induced Plasmon Decay. Journal of Physical Chemistry C, 2017, 121, 15368-15374.	1.5	24
111	Mixed Cation FA_xPEA_{1â€“}_xPbI₃ with Enhanced Phase and Ambient Stability toward Highâ€Performance Perovskite Solar Cells. Advanced Energy Materials, 2017, 7, 1601307.	10.2	298
112	Real time propagation of the exact two component time-dependent density functional theory. Journal of Chemical Physics, 2016, 145, 104107.	1.2	71
113	Can Quantized Vibrational Effects Be Obtained from Ehrenfest Mixed Quantum-Classical Dynamics?. Journal of Physical Chemistry Letters, 2016, 7, 5193-5197.	2.1	6
114	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.	1.2	41
115	Relativistic Two-Component Particleâ€“Particle Tammâ€“Dancoff Approximation. Journal of Chemical Theory and Computation, 2016, 12, 5379-5384.	2.3	13
116	Imaging ultrafast excited state pathways in transition metal complexes by X-ray transient absorption and scattering using X-ray free electron laser source. Faraday Discussions, 2016, 194, 639-658.	1.6	10
117	Quantum confinement effects on optical transitions in nanodiamonds containing nitrogen vacancies. Physical Review B, 2016, 94, .	1.1	36
118	â€œWatchingâ€•Polaron Pair Formation from First-Principles Electronâ€“Nuclear Dynamics. Journal of Physical Chemistry A, 2016, 120, 7255-7261.	1.1	47
119	Classical or Quantum? A Computational Study of Small Ion Diffusion in IIâ€“VI Semiconductor Quantum Dots. Journal of Physical Chemistry C, 2016, 120, 19434-19441.	1.5	16
120	Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures. Journal of Chemical Theory and Computation, 2016, 12, 3711-3718.	2.3	51
121	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.	2.3	18
122	Ab Initio Transient Vibrational Spectral Analysis. Journal of Physical Chemistry Letters, 2016, 7, 4501-4508.	2.1	37
123	Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy. Journal of the American Chemical Society, 2016, 138, 8752-8764.	6.6	77
124	Single-Crystal and Electronic Structure of a 1.3 nm Indium Phosphide Nanocluster. Journal of the American Chemical Society, 2016, 138, 1510-1513.	6.6	164
125	Computational Studies of the Electronic Structures of Copper-Doped CdSe Nanocrystals: Oxidation States, Jahnâ€“Teller Distortions, Vibronic Bandshapes, and Singletâ€“Triplet Splittings. Journal of Physical Chemistry C, 2016, 120, 5714-5723.	1.5	63
126	Direct ab Initio (Meta-)Surface-Hopping Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 935-945.	2.3	40

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127	Approximate singly excited states from a two-component Hartree-Fock reference. Journal of Chemical Physics, 2015, 143, 144106.	1.2	10
128	The consequences of improperly describing oscillator strengths beyond the electric dipole approximation. Journal of Chemical Physics, 2015, 143, 234103.	1.2	34
129	Ab initio two-component Ehrenfest dynamics. Journal of Chemical Physics, 2015, 143, 114105.	1.2	31
130	Imaging Excited Orbitals of Quantum Dots: Experiment and Electronic Structure Theory. Journal of the American Chemical Society, 2015, 137, 14743-14750.	6.6	18
131	Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements. Journal of Chemical Theory and Computation, 2015, 11, 2994-2999.	2.3	78
132	Stability of the complex generalized Hartree-Fock equations. Journal of Chemical Physics, 2015, 142, 154109.	1.2	29
133	Real-Time TDDFT Studies of Exciton Decay and Transfer in Silver Nanowire Arrays. Journal of Physical Chemistry C, 2015, 119, 6421-6427.	1.5	46
134	A conductive liquid crystal via facile doping of an n-type benzodifurandione derivative. Journal of Materials Chemistry A, 2015, 3, 6929-6934.	5.2	14
135	Time-dependent non-equilibrium dielectric response in QM/continuum approaches. Journal of Chemical Physics, 2015, 142, 034120.	1.2	31
136	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, 4146-4153.	2.3	92
137	Assessment of low-scaling approximations to the equation of motion coupled-cluster singles and doubles equations. Journal of Chemical Physics, 2014, 141, 164116.	1.2	45
138	Ferromagnetic excited-state Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math>dimers in Zn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Mnx quantum dots observed by time-resolved magnetophotoluminescence. Physical Review B, 2014, 89, .	1.1	40
139	Quantum coherent plasmon in silver nanowires: A real-time TDDFT study. Journal of Chemical Physics, 2014, 140, 244705.	1.2	57
140	Ab initio non-relativistic spin dynamics. Journal of Chemical Physics, 2014, 141, 214111.	1.2	20
141	Dynamical Investigations of Inhomogeneous Vibrational Broadening in Diluted Magnetic Semiconductor Nanocrystals. Journal of Physical Chemistry C, 2014, 118, 3266-3273.	1.5	6
142	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.	1.5	31
143	Non-adiabatic molecular dynamics investigation of photoionization state formation and lifetime in Mn²⁺-doped ZnO quantum dots. Physical Chemistry Chemical Physics, 2014, 16, 17507.	1.3	24
144	Effect of Excited-State Structural Relaxation on Midgap Excitations in Co²⁺-Doped ZnO Quantum Dots. Journal of Physical Chemistry C, 2014, 118, 13152-13156.	1.5	19

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145	From charge-transfer to a charge-separated state: a perspective from the real-time TDDFT excitonic dynamics. Physical Chemistry Chemical Physics, 2014, 16, 24457-24465.	1.3	51
146	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.	1.5	13
147	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, 3933-3938.	2.3	24
148	An efficient method for calculating dynamical hyperpolarizabilities using real-time time-dependent density functional theory. Journal of Chemical Physics, 2013, 138, 064104.	1.2	72
149	Solvent Effects on Intramolecular Charge Transfer Dynamics in a Fullerene Derivative. Journal of Physical Chemistry A, 2013, 117, 2687-2691.	1.1	22
150	Doping of Fullerenes via Anionâ€Induced Electron Transfer and Its Implication for Surfactant Facilitated High Performance Polymer Solar Cells. Advanced Materials, 2013, 25, 4425-4430.	11.1	244
151	Solutionâ€Processible Highly Conducting Fullerenes. Advanced Materials, 2013, 25, 2457-2461.	11.1	130
152	Modeling Ultrafast Solvated Electronic Dynamics Using Time-Dependent Density Functional Theory and Polarizable Continuum Model. Journal of Physical Chemistry A, 2012, 116, 1884-1890.	1.1	27
153	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.	2.1	40
154	Ferromagnetism in p-Type Manganese-Doped Zinc Oxide Quantum Dots. Journal of Physical Chemistry Letters, 2012, 3, 1374-1380.	2.1	21
155	Mechanisms of bridge-mediated electron transfer: A TDDFT electronic dynamics study. Journal of Chemical Physics, 2012, 137, 22A512.	1.2	22
156	Orbital pathways for Mn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math>-carrier<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:mi>p</mml:mi><mml:mo>â^’</mml:mo><mml:mi>d</mml:mi></mml:mrow><in diluted magnetic semiconductor quantum dots. Physical Review B, 2011, 84, .	1.1	56
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