Oleg Prezhdo

List of Publications by Year
in descending order

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483 papers	25,492 citations	4146 87 h-index	11308 136 g-index
495 all docs	495 docs citations	495 times ranked	16728 citing authors

#	Article	IF	Citations
1	Trajectory Surface Hopping in the Time-Dependent Kohn-Sham Approach for Electron-Nuclear Dynamics. Physical Review Letters, 2005, 95, 163001.	7.8	611
2	The PYXAID Program for Non-Adiabatic Molecular Dynamics in Condensed Matter Systems. Journal of Chemical Theory and Computation, 2013, 9, 4959-4972.	5.3	588
3	Theoretical Studies of Photoinduced Electron Transfer in Dye-Sensitized TiO2. Annual Review of Physical Chemistry, 2007, 58, 143-184.	10.8	534
4	Decoherence-induced surface hopping. Journal of Chemical Physics, 2012, 137, 22A545.	3.0	491
5	Advanced Capabilities of the PYXAID Program: Integration Schemes, Decoherence Effects, Multiexcitonic States, and Field-Matter Interaction. Journal of Chemical Theory and Computation, 2014, 10, 789-804.	5.3	472
6	Theoretical Insights into Photoinduced Charge Transfer and Catalysis at Oxide Interfaces. Chemical Reviews, 2013, 113, 4496-4565.	47.7	455
7	Unravelling the Effects of Grain Boundary and Chemical Doping on Electronâ€“Hole Recombination in CH₃NH₃PbI₃ Perovskite by Time-Domain Atomistic Simulation. Journal of the American Chemical Society, 2016, 138, 3884-3890.	13.7	333
8	Quantum decoherence and the isotope effect in condensed phase nonadiabatic molecular dynamics simulations. Journal of Chemical Physics, 1996, 104, 5942-5955.	3.0	331
9	Mean-field molecular dynamics with surface hopping. Journal of Chemical Physics, 1997, 107, 825-834.	3.0	306
10	Evaluation of quantum transition rates from quantum-classical molecular dynamics simulations. Journal of Chemical Physics, 1997, 107, 5863-5878.	3.0	299
11	Recent Progress in Surface Hopping: 2011â€“2015. Journal of Physical Chemistry Letters, 2016, 7, 2100-2112.	4.6	279
12	AbInitioNonadiabatic Molecular Dynamics of the Ultrafast Electron Injection across the Alizarinâ^'TiO2Interface. Journal of the American Chemical Society, 2005, 127, 7941-7951.	13.7	261
13	Detection of Nucleic Acids with Graphene Nanopores: Ab Initio Characterization of a Novel Sequencing Device. Nano Letters, 2010, 10, 3237-3242.	9.1	247
14	Breaking the Phonon Bottleneck in PbSe and CdSe Quantum Dots: Time-Domain Density Functional Theory of Charge Carrier Relaxation. ACS Nano, 2009, 3, 93-99.	14.6	236
15	Ultrafast Carrier Thermalization and Cooling Dynamics in Few-Layer MoS₂. ACS Nano, 2014, 8, 10931-10940.	14.6	236
16	Quantum Zeno Effect Rationalizes the Phonon Bottleneck in Semiconductor Quantum Dots. Physical Review Letters, 2013, 110, 180404.	7.8	230
17	Photo-induced Charge Separation across the Grapheneâ€“TiO₂ Interface Is Faster than Energy Losses: A Time-Domain ab Initio Analysis. Journal of the American Chemical Society, 2012, 134, 14238-14248.	13.7	226
18	Quantum Coherence Facilitates Efficient Charge Separation at a MoS₂/MoSe₂ van der Waals Junction. Nano Letters, 2016, 16, 1996-2003.	9.1	225

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19	Instantaneous Generation of Charge-Separated State on TiO₂ Surface Sensitized with Plasmonic Nanoparticles. Journal of the American Chemical Society, 2014, 136, 4343-4354.	13.7	221
20	Time-Domainab InitioStudy of Charge Relaxation and Recombination in Dye-Sensitized TiO2. Journal of the American Chemical Society, 2007, 129, 8528-8543.	13.7	207
21	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. Nano Letters, 2017, 17, 6435-6442.	9.1	204
22	Colloidal Semiconductor Quantum Dots with Tunable Surface Composition. Nano Letters, 2012, 12, 4465-4471.	9.1	201
23	Shape-controlled synthesis of silver nanoparticles: Ab initio study of preferential surface coordination with citric acid. Chemical Physics Letters, 2008, 458, 113-116.	2.6	199
24	Auger-Assisted Electron Transfer from Photoexcited Semiconductor Quantum Dots. Nano Letters, 2014, 14, 1263-1269.	9.1	197
25	Relationship between Quantum Decoherence Times and Solvation Dynamics in Condensed Phase Chemical Systems. Physical Review Letters, 1998, 81, 5294-5297.	7.8	193
26	Electronic Structure and Spectra of Catechol and Alizarin in the Gas Phase and Attached to Titanium. Journal of Physical Chemistry B, 2005, 109, 365-373.	2.6	188
27	Mixing quantum and classical mechanics. Physical Review A, 1997, 56, 162-175.	2.5	187
28	The Two-Pathway Model for the Catch-Slip Transition in Biological Adhesion. Biophysical Journal, 2005, 89, 1446-1454.	0.5	186
29	Large-Scale Computations in Chemistry: A Birdâ€™s Eye View of a Vibrant Field. Chemical Reviews, 2015, 115, 5797-5890.	47.7	182
30	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. Science Advances, 2020, 6, eaaw7453.	10.3	182
31	Nonadiabatic Molecular Dynamics Simulation of Light-Induced Electron Transfer from an Anchored Molecular Electron Donor to a Semiconductor Acceptorâ€. Journal of Physical Chemistry B, 2002, 106, 8047-8054.	2.6	180
32	Regarding the validity of the time-dependent Kohnâ€“Sham approach for electron-nuclear dynamics via trajectory surface hopping. Journal of Chemical Physics, 2011, 134, 024102.	3.0	178
33	Photoinduced electron dynamics at the chromophoreâ€“semiconductor interface: A time-domain ab initio perspective. Progress in Surface Science, 2009, 84, 30-68.	8.3	168
34	Persistent Electronic Coherence Despite Rapid Loss of Electronâ€“Nuclear Correlation. Journal of Physical Chemistry Letters, 2013, 4, 3857-3864.	4.6	165
35	Mean field approximation for the stochastic SchrÃ¶dinger equation. Journal of Chemical Physics, 1999, 111, 8366-8377.	3.0	158
36	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. ACS Energy Letters, 2017, 2, 1270-1278.	17.4	151

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37	A Simple Solution to the Trivial Crossing Problem in Surface Hopping. Journal of Physical Chemistry Letters, 2014, 5, 713-719.	4.6	148
38	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie - International Edition, 2020, 59, 6435-6441.	13.8	147
39	Quantum Backreaction through the Bohmian Particle. Physical Review Letters, 2001, 86, 3215-3219.	7.8	146
40	Nonadiabatic Dynamics of Charge Transfer and Singlet Fission at the Pentacene/C₆₀ Interface. Journal of the American Chemical Society, 2014, 136, 1599-1608.	13.7	142
41	Scanning Tunneling Microscopy of DNA-Wrapped Carbon Nanotubes. Nano Letters, 2009, 9, 12-17.	9.1	140
42	Moderate Humidity Delays Electronâ€“Hole Recombination in Hybrid Organicâ€“Inorganic Perovskites: Time-Domain Ab Initio Simulations Rationalize Experiments. Journal of Physical Chemistry Letters, 2016, 7, 3215-3222.	4.6	139
43	Acetonitrile Boosts Conductivity of Imidazolium Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 7719-7727.	2.6	136
44	Sulfur Adatom and Vacancy Accelerate Charge Recombination in MoS₂ but by Different Mechanisms: Time-Domain Ab Initio Analysis. Nano Letters, 2017, 17, 7962-7967.	9.1	136
45	Maximizing Singlet Fission by Intermolecular Packing. Journal of Physical Chemistry Letters, 2014, 5, 3345-3353.	4.6	135
46	Donorâ€“Acceptor Interaction Determines the Mechanism of Photoinduced Electron Injection from Graphene Quantum Dots into TiO₂: Ï€-Stacking Supersedes Covalent Bonding. Journal of the American Chemical Society, 2017, 139, 2619-2629.	13.7	132
47	Control of Charge Carriers Trapping and Relaxation in Hematite by Oxygen Vacancy Charge: Ab Initio Non-adiabatic Molecular Dynamics. Journal of the American Chemical Society, 2017, 139, 6707-6717.	13.7	132
48	Control of Charge Recombination in Perovskites by Oxidation State of Halide Vacancy. Journal of the American Chemical Society, 2018, 140, 15753-15763.	13.7	129
49	Surface Ligands Increase Photoexcitation Relaxation Rates in CdSe Quantum Dots. ACS Nano, 2012, 6, 6515-6524.	14.6	128
50	Charge Separation and Recombination in Two-Dimensional MoS₂/WS₂: Time-Domain ab Initio Modeling. Chemistry of Materials, 2017, 29, 2466-2473.	6.7	127
51	Nonradiative Quenching of Fluorescence in a Semiconducting Carbon Nanotube: A Time-DomainAbÂInitioStudy. Physical Review Letters, 2008, 100, 197402.	7.8	126
52	Ultrafast Dynamics of Photongenerated Holes at a CH₃OH/TiO₂ Rutile Interface. Journal of the American Chemical Society, 2016, 138, 13740-13749.	13.7	126
53	Global Flux Surface Hopping Approach for Mixed Quantum-Classical Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 3598-3605.	5.3	125
54	Photoinduced Dynamics in Semiconductor Quantum Dots: Insights from Time-Domain ab Initio Studies. Accounts of Chemical Research, 2009, 42, 2005-2016.	15.6	124

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55	Dynamics of the Photoexcited Electron at the Chromophoreâ€“Semiconductor Interface. Accounts of Chemical Research, 2008, 41, 339-348.	15.6	123
56	Time-Domain Ab Initio Modeling of Photoinduced Dynamics at Nanoscale Interfaces. Annual Review of Physical Chemistry, 2015, 66, 549-579.	10.8	121
57	Guestâ^'Host Cooperativity in Organic Materials Greatly Enhances the Nonlinear Optical Response. Journal of Physical Chemistry C, 2008, 112, 4355-4363.	3.1	120
58	Ab Initio Nonadiabatic Molecular Dynamics of the Ultrafast Electron Injection from a PbSe Quantum Dot into the TiO₂ Surface. Journal of the American Chemical Society, 2011, 133, 19240-19249.	13.7	120
59	Phonon-Induced Dephasing of Excitons in Semiconductor Quantum Dots: Multiple Exciton Generation, Fission, and Luminescence. ACS Nano, 2009, 3, 2487-2494.	14.6	115
60	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain Ab Initio Analysis. Nano Letters, 2018, 18, 2459-2466.	9.1	114
61	Spinâ€“Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. ACS Energy Letters, 2018, 3, 2159-2166.	17.4	114
62	Quantum Anti-Zeno Acceleration of a Chemical Reaction. Physical Review Letters, 2000, 85, 4413-4417.	7.8	112
63	Ab Initio Time-Domain Study of Phonon-Assisted Relaxation of Charge Carriers in a PbSe Quantum Dot. Journal of Physical Chemistry C, 2007, 111, 4871-4878.	3.1	108
64	Water Boiling Inside Carbon Nanotubes: Toward Efficient Drug Release. ACS Nano, 2011, 5, 5647-5655.	14.6	108
65	Dopants Control Electronâ€“Hole Recombination at Perovskiteâ€“TiO₂ Interfaces: Ab Initio Time-Domain Study. ACS Nano, 2015, 9, 11143-11155.	14.6	108
66	Quantized Hamilton dynamics. Journal of Chemical Physics, 2000, 113, 6557-6565.	3.0	107
67	Nonadiabatic Dynamics of Positive Charge during Photocatalytic Water Splitting on GaN(10-10) Surface: Charge Localization Governs Splitting Efficiency. Journal of the American Chemical Society, 2013, 135, 8682-8691.	13.7	107
68	What Makes the Photocatalytic CO₂ Reduction on N-Doped Ta₂O₅ Efficient: Insights from Nonadiabatic Molecular Dynamics. Journal of the American Chemical Society, 2015, 137, 11517-11525.	13.7	105
69	Ionic and Molecular Liquids: Working Together for Robust Engineering. Journal of Physical Chemistry Letters, 2013, 4, 1423-1431.	4.6	103
70	Chlorine Doping Reduces Electronâ€“Hole Recombination in Lead Iodide Perovskites: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2015, 6, 4463-4469.	4.6	103
71	Halide Composition Controls Electronâ€“Hole Recombination in Cesiumâ€“Lead Halide Perovskite Quantum Dots: A Time Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2018, 9, 1872-1879.	4.6	103
72	Superoxide/Peroxide Chemistry Extends Charge Carriersâ€™ Lifetime but Undermines Chemical Stability of CH₃NH₃PbI₃ Exposed to Oxygen: Time-Domain ab Initio Analysis. Journal of the American Chemical Society, 2019, 141, 5798-5807.	13.7	102

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73	Ab Initio Nonadiabatic Molecular Dynamics of Wet-Electrons on the TiO₂ Surface. Journal of the American Chemical Society, 2009, 131, 15483-15491.	13.7	99
74	Exciton Dissociation and Suppressed Charge Recombination at 2D Perovskite Edges: Key Roles of Unsaturated Halide Bonds and Thermal Disorder. Journal of the American Chemical Society, 2019, 141, 15557-15566.	13.7	98
75	Quantized Hamilton Dynamics. Theoretical Chemistry Accounts, 2006, 116, 206-218.	1.4	96
76	Ab Initio Study of Vibrational Dephasing of Electronic Excitations in Semiconducting Carbon Nanotubes. Nano Letters, 2007, 7, 3260-3265.	9.1	96
77	Temperature Independence of the Photoinduced Electron Injection in Dye-Sensitized TiO₂ Rationalized by Ab Initio Time-Domain Density Functional Theory. Journal of the American Chemical Society, 2008, 130, 9756-9762.	13.7	96
78	Time-DomainAbÂInitioSimulation of Electron and Hole Relaxation Dynamics in a Single-Wall Semiconducting Carbon Nanotube. Physical Review Letters, 2006, 96, 187401.	7.8	95
79	Why Chemical Vapor Deposition Grown MoS₂ Samples Outperform Physical Vapor Deposition Samples: Time-Domain ab Initio Analysis. Nano Letters, 2018, 18, 4008-4014.	9.1	94
80	Thermally Assisted Sub-10â€‰fs Electron Transfer in Dye-Sensitized Nanocrystalline TiO2 Solar Cells. Advanced Materials, 2004, 16, 240-244.	21.0	93
81	Generation of Multiple Excitons in PbSe and CdSe Quantum Dots by Direct Photoexcitation: First-Principles Calculations on Small PbSe and CdSe Clusters. Journal of Physical Chemistry C, 2008, 112, 18291-18294.	3.1	93
82	Time-Domain ab Initio Study of Auger and Phonon-Assisted Auger Processes in a Semiconductor Quantum Dot. Nano Letters, 2011, 11, 1845-1850.	9.1	93
83	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. Journal of Chemical Theory and Computation, 2016, 12, 1436-1448.	5.3	93
84	Multiple excitons and the electronâ€“phonon bottleneck in semiconductor quantum dots: An ab initio perspective. Chemical Physics Letters, 2008, 460, 1-9.	2.6	92
85	Isomerization of all-trans-Retinol to cis-Retinols in Bovine Retinal Pigment Epithelial Cells:â€‰Dependence on the Specificity of Retinoid-Binding Proteins. Biochemistry, 2000, 39, 11370-11380.	2.5	91
86	Multiple Exciton Generation and Recombination Dynamics in Small Si and CdSe Quantum Dots: An Ab Initio Time-Domain Study. ACS Nano, 2012, 6, 1239-1250.	14.6	91
87	Synergy between Ion Migration and Charge Carrier Recombination in Metal-Halide Perovskites. Journal of the American Chemical Society, 2020, 142, 3060-3068.	13.7	91
88	Covalent Linking Greatly Enhances Photoinduced Electron Transfer in Fullerene-Quantum Dot Nanocomposites: Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2013, 4, 1-6.	4.6	90
89	Lewis Base Passivation of Hybrid Halide Perovskites Slows Electronâ€“Hole Recombination: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 1164-1171.	4.6	90
90	Ab Initio Study of Temperature and Pressure Dependence of Energy and Phonon-Induced Dephasing of Electronic Excitations in CdSe and PbSe Quantum Dots. Journal of Physical Chemistry C, 2008, 112, 7800-7808.	3.1	89

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91	Ultrafast Vibrationally-Induced Dephasing of Electronic Excitations in PbSe Quantum Dots. Nano Letters, 2006, 6, 2295-2300.	9.1	88
92	Coherence penalty functional: A simple method for adding decoherence in Ehrenfest dynamics. Journal of Chemical Physics, 2014, 140, 194107.	3.0	86
93	Delocalized Impurity Phonon Induced Electronâ€“Hole Recombination in Doped Semiconductors. Nano Letters, 2018, 18, 1592-1599.	9.1	86
94	Mixed quantum-classical dynamics for charge transport in organics. Physical Chemistry Chemical Physics, 2015, 17, 12395-12406.	2.8	85
95	Solvent Mode Participation in the Nonradiative Relaxation of the Hydrated Electron. The Journal of Physical Chemistry, 1996, 100, 17094-17102.	2.9	83
96	Theoretical Aspects of the Biological Catch Bond. Accounts of Chemical Research, 2009, 42, 693-703.	15.6	82
97	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. Physical Review B, 2018, 97, .	3.2	81
98	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. Angewandte Chemie - International Edition, 2020, 59, 4684-4690.	13.8	78
99	Aromaticity indices revisited: refinement and application to certain five-membered ring heterocycles. Tetrahedron, 2001, 57, 5715-5729.	1.9	77
100	Mono-Elemental Properties of 2D Black Phosphorus Ensure Extended Charge Carrier Lifetimes under Oxidation: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 1083-1091.	4.6	74
101	Nonadiabatic charge dynamics in novel solar cell materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1305.	14.6	71
102	Optoelectronic Properties of Semiconductor Quantum Dot Solids for Photovoltaic Applications. Journal of Physical Chemistry Letters, 2017, 8, 4129-4139.	4.6	71
103	Plasmon-Mediated Electron Injection from Au Nanorods into MoS2: Traditional versus Photoexcitation Mechanism. CheM, 2018, 4, 1112-1127.	11.7	71
104	Heat-Driven Release of a Drug Molecule from Carbon Nanotubes: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 13481-13486.	2.6	70
105	Interplay between Localized and Free Charge Carriers Can Explain Hot Fluorescence in the CH3NH3PbBr3 Perovskite: Time-Domain Ab Initio Analysis. Journal of the American Chemical Society, 2017, 139, 17327-17333.	13.7	70
106	Ab initio nonadiabatic molecular dynamics of charge carriers in metal halide perovskites. Nanoscale, 2021, 13, 10239-10265.	5.6	70
107	Strong Interaction at the Perovskite/TiO₂ Interface Facilitates Ultrafast Photoinduced Charge Separation: A Nonadiabatic Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 3797-3806.	3.1	69
108	Role of Methylammonium Orientation in Ion Diffusion and Currentâ€“Voltage Hysteresis in the CH₃NH₃PbI₃ Perovskite. ACS Energy Letters, 2017, 2, 1997-2004.	17.4	68

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109	Time-Domain ab Initio Analysis Rationalizes the Unusual Temperature Dependence of Charge Carrier Relaxation in Lead Halide Perovskite. ACS Energy Letters, 2018, 3, 2713-2720.	17.4	68
110	Increased Lattice Stiffness Suppresses Nonradiative Charge Recombination in MAPbI₃ Doped with Larger Cations: Time-Domain Ab Initio Analysis. ACS Energy Letters, 2018, 3, 2070-2076.	17.4	68
111	Ab initio study of exciton transfer dynamics from a coreâ€“shell semiconductor quantum dot to a porphyrin-sensitizer. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 342-351.	3.9	67
112	Asymmetry in the Electron and Hole Transfer at a Polymerâ€“Carbon Nanotube Heterojunction. Nano Letters, 2014, 14, 3335-3341.	9.1	67
113	Understanding Hematite Doping with Group IV Elements: A DFT+U Study. Journal of Physical Chemistry C, 2015, 119, 26303-26310.	3.1	66
114	Anharmonicity Extends Carrier Lifetimes in Lead Halide Perovskites at Elevated Temperatures. Journal of Physical Chemistry Letters, 2019, 10, 6219-6226.	4.6	66
115	Influence of Defects on Excited-State Dynamics in Lead Halide Perovskites: Time-Domain ab Initio Studies. Journal of Physical Chemistry Letters, 2019, 10, 3788-3804.	4.6	66
116	Ab Initio Time-Domain Study of the Triplet State in a Semiconducting Carbon Nanotube: Intersystem Crossing, Phosphorescence Time, and Line Width. Journal of the American Chemical Society, 2012, 134, 15648-15651.	13.7	65
117	Nanoscale Carbon Greatly Enhances Mobility of a Highly Viscous Ionic Liquid. ACS Nano, 2014, 8, 8190-8197.	14.6	65
118	Symmetry Breaking at MAPbI₃ Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 1617-1623.	4.6	65
119	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	4.6	65
120	Tunable Hydrogen Doping of Metal Oxide Semiconductors with Acidâ€“Metal Treatment at Ambient Conditions. Journal of the American Chemical Society, 2020, 142, 4136-4140.	13.7	65
121	Why Oxygen Increases Carrier Lifetimes but Accelerates Degradation of CH₃NH₃PbI₃ under Light Irradiation: Time-Domain Ab Initio Analysis. Journal of the American Chemical Society, 2020, 142, 14664-14673.	13.7	64
122	Minimizing Electronâ€“Hole Recombination on TiO₂ Sensitized with PbSe Quantum Dots: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2014, 5, 2941-2946.	4.6	63
123	CO₂ Photoreduction on Metal Oxide Surface Is Driven by Transient Capture of Hot Electrons: Ab Initio Quantum Dynamics Simulation. Journal of the American Chemical Society, 2020, 142, 3214-3221.	13.7	63
124	Suppression of Electronâ€“Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. Journal of Physical Chemistry Letters, 2019, 10, 6151-6158.	4.6	62
125	Uniform Diffusion of Acetonitrile inside Carbon Nanotubes Favors Supercapacitor Performance. Nano Letters, 2008, 8, 2126-2130.	9.1	61
126	Defects Are Needed for Fast Photo-Induced Electron Transfer from a Nanocrystal to a Molecule: Time-Domain Ab Initio Analysis. Journal of the American Chemical Society, 2013, 135, 18892-18900.	13.7	61

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127	Theoretical Study of Electronâ€“Phonon Relaxation in PbSe and CdSe Quantum Dots: Evidence for Phonon Memory. Journal of Physical Chemistry C, 2011, 115, 21641-21651.	3.1	60
128	Fewest Switches Surface Hopping in Liouville Space. Journal of Physical Chemistry Letters, 2015, 6, 3827-3833.	4.6	60
129	Lattice Expansion in Hybrid Perovskites: Effect on Optoelectronic Properties and Charge Carrier Dynamics. Journal of Physical Chemistry Letters, 2019, 10, 5000-5007.	4.6	60
130	Confinement by Carbon Nanotubes Drastically Alters the Boiling and Critical Behavior of Water Droplets. ACS Nano, 2012, 6, 2766-2773.	14.6	59
131	Ligands Slow Down Pure-Dephasing in Semiconductor Quantum Dots. ACS Nano, 2015, 9, 9106-9116.	14.6	59
132	Microscopic Structure and Dynamics of LiBF₄ Solutions in Cyclic and Linear Carbonates. Journal of Physical Chemistry B, 2011, 115, 14563-14571.	2.6	58
133	Nonadiabatic Ensemble Simulations of cis-Stilbene and cis-Azobenzene Photoisomerization. Journal of Chemical Theory and Computation, 2014, 10, 14-23.	5.3	58
134	Water Splitting with a Single-Atom Cu/TiO₂ Photocatalyst: Atomistic Origin of High Efficiency and Proposed Enhancement by Spin Selection. Jacs Au, 2021, 1, 550-559.	7.9	58
135	A new force field model of 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid and acetonitrile mixtures. Physical Chemistry Chemical Physics, 2011, 13, 19345.	2.8	57
136	Auger-Mediated Electron Relaxation Is Robust to Deep Hole Traps: Time-Domain Ab Initio Study of CdSe Quantum Dots. Nano Letters, 2015, 15, 2086-2091.	9.1	57
137	Quantized Hamilton dynamics for a general potential. Journal of Chemical Physics, 2002, 116, 4450-4461.	3.0	56
138	Structural Deformation Controls Charge Losses in MAPbI₃: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2020, 5, 1930-1938.	17.4	55
139	Classical mapping for second-order quantized Hamiltonian dynamics. Journal of Chemical Physics, 2002, 117, 2995-3002.	3.0	54
140	Long Carrier Lifetimes in PbI₂-Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2018, 3, 1868-1874.	17.4	54
141	Protecting hot carriers by tuning hybrid perovskite structures with alkali cations. Science Advances, 2020, 6, .	10.3	54
142	Iodine and Sulfur Vacancy Cooperation Promotes Ultrafast Charge Extraction at MAPbI₃/MoS₂ Interface. ACS Energy Letters, 2020, 5, 1346-1354.	17.4	53
143	DFT Simulation and Vibrational Analysis of the IR and Raman Spectra of a CdSe Quantum Dot Capped by Methylamine and Trimethylphosphine Oxide Ligands. Journal of Physical Chemistry C, 2012, 116, 14674-14681.	3.1	52
144	Ferroelectric Alignment of Organic Cations Inhibits Nonradiative Electronâ€“Hole Recombination in Hybrid Perovskites: Ab Initio Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 812-818.	4.6	52

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145	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. Journal of the American Chemical Society, 2021, 143, 9982-9990.	13.7	52
146	Quantized mean-field approximation. Chemical Physics Letters, 2001, 346, 463-469.	2.6	50
147	Macroscopic Order and Electro-Optic Response of Dipolar Chromophore-Polymer Materials. ChemPhysChem, 2004, 5, 1821-1830.	2.1	50
148	Force-induced deformations and stability of biological bonds. Physical Review E, 2006, 73, 050902.	2.1	50
149	Virtual Issue: Graphene and Functionalized Graphene. Journal of Physical Chemistry C, 2011, 115, 3195-3197.	3.1	50
150	Nitrogenâ€“Nitrogen Bonds Undermine Stability of N-Doped Graphene. Journal of the American Chemical Society, 2015, 137, 11688-11694.	13.7	49
151	Nonadiabatic Molecular Dynamics Study of Electron Transfer from Alizarin to the Hydrated Ti4+ Ion. Journal of Physical Chemistry B, 2005, 109, 17998-18002.	2.6	48
152	Recent theoretical progress in the development of perovskite photovoltaic materials. Journal of Energy Chemistry, 2018, 27, 637-649.	12.9	48
153	Advancing Physical Chemistry with Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 9656-9658.	4.6	48
154	Ultrafast Electron and Hole Relaxation Pathways in Few-Layer MoS₂. Journal of Physical Chemistry C, 2015, 119, 20698-20708.	3.1	47
155	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. ACS Energy Letters, 2020, 5, 3813-3820.	17.4	47
156	Symmetric band structures and asymmetric ultrafast electron and hole relaxations in silicon and germanium quantum dots: time-domain ab initio simulation. Dalton Transactions, 2009, , 10069.	3.3	46
157	Time-Domain Ab Initio Study of Phonon-Induced Relaxation of Plasmon Excitations in a Silver Quantum Dot. Journal of Physical Chemistry C, 2012, 116, 15034-15040.	3.1	46
158	Long-Lived Hot Electron in a Metallic Particle for Plasmonics and Catalysis: Ab Initio Nonadiabatic Molecular Dynamics with Machine Learning. ACS Nano, 2020, 14, 10608-10615.	14.6	46
159	Phonon-Mediated Interlayer Charge Separation and Recombination in a MoSe₂/WSe₂ Heterostructure. Nano Letters, 2021, 21, 2165-2173.	9.1	46
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