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	Efficient passivation of DY center in CH3NH3PbBr3 by chlorine: Quantum molecular dynamics. Nano Research, 2022, 15, 2112-2122.	10.4	28
2	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Inverse Fast Fourier Transform. Journal of Physical Chemistry Letters, 2022, 13, 331-338.	4.6	8
3	Excited State Dynamics in Dual-Defects Modified Graphitic Carbon Nitride. Journal of Physical Chemistry Letters, 2022, 13, 1033-1041.	4.6	16
4	Dimensionality reduction in machine learning for nonadiabatic molecular dynamics: Effectiveness of elemental sublattices in lead halide perovskites. Journal of Chemical Physics, 2022, 156, 054110.	3.0	4
5	The twist angle has weak influence on charge separation and strong influence on recombination in the MoS₂/WS₂ bilayer: ab initio quantum dynamics. Journal of Materials Chemistry A, 2022, 10, 8324-8333.	10.3	30
6	Charge carrier nonadiabatic dynamics in non-metal doped graphitic carbon nitride. Journal of Chemical Physics, 2022, 156, 094702.	3.0	22
7	Suppressing Oxygen-Induced Deterioration of Metal Halide Perovskites by Alkaline Earth Metal Doping: A Quantum Dynamics Study. Journal of the American Chemical Society, 2022, 144, 5543-5551.	13.7	29
8	How Hole Injection Accelerates Both Ion Migration and Nonradiative Recombination in Metal Halide Perovskites. Journal of the American Chemical Society, 2022, 144, 6604-6612.	13.7	31
9	Chemical passivation of methylammonium fragments eliminates traps, extends charge lifetimes, and restores structural stability of CH3NH3PbI3 perovskite. Nano Research, 2022, 15, 4765-4772.	10.4	12
10	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO₂(110) Surface. Jacs Au, 2022, 2, 234-245.	7.9	22
11	Agâ€“Bi Charge Redistribution Creates Deep Traps in Defective Cs₂AgBiBr₆: Machine Learning Analysis of Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 3645-3651.	4.6	18
12	Point Defects in Two-Dimensional Ruddlesdenâ€“Popper Perovskites Explored with Ab Initio Calculations. Journal of Physical Chemistry Letters, 2022, 13, 5213-5219.	4.6	11
13	Electron-Volt Fluctuation of Defect Levels in Metal Halide Perovskites on a 100 ps Time Scale. Journal of Physical Chemistry Letters, 2022, 13, 5946-5952.	4.6	18
14	Adsorption of Lanthanide Atoms on Graphene: Similar, Yet Different. Journal of Physical Chemistry Letters, 2022, 13, 6042-6047.	4.6	5
15	Ultrafast charge transfer coupled to quantum proton motion at molecule/metal oxide interface. Science Advances, 2022, 8, .	10.3	21
16	Electronâ€“phonon relaxation at the Au/WSe₂ interface is significantly accelerated by a Ti adhesion layer: time-domain ab initio analysis. Nanoscale, 2022, 14, 10514-10523.	5.6	7
17	Long-lived modulation of plasmonic absorption by ballistic thermal injection. Nature Nanotechnology, 2021, 16, 47-51.	31.5	40
18	Bidentate Lewis bases are preferred for passivation of MAPbI3 surfaces: A time-domain ab initio analysis. Nano Energy, 2021, 79, 105491.	16.0	33

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19	Modeling Auger Processes with Nonadiabatic Molecular Dynamics. Nano Letters, 2021, 21, 756-761.	9.1	29
20	Weak Distance Dependence of Hot-Electron-Transfer Rates at the Interface between Monolayer MoS₂ and Gold. ACS Nano, 2021, 15, 819-828.	14.6	27
21	Ab initio nonadiabatic molecular dynamics of charge carriers in metal halide perovskites. Nanoscale, 2021, 13, 10239-10265.	5.6	70
22	Tuning charge transfer and recombination in exTTF/CNT nanohybrids by choice of chalcogen: A time-domain density functional analysis. Journal of Applied Physics, 2021, 129, .	2.5	9
23	Atomistic Mechanism of Passivation of Halide Vacancies in Lead Halide Perovskites by Alkali Ions. Chemistry of Materials, 2021, 33, 1285-1292.	6.7	26
24	Phonon-Mediated Interlayer Charge Separation and Recombination in a MoSe₂/WSe₂ Heterostructure. Nano Letters, 2021, 21, 2165-2173.	9.1	46
25	Chemically Switchable n-Type and p-Type Conduction in Bismuth Selenide Nanoribbons for Thermoelectric Energy Harvesting. ACS Nano, 2021, 15, 2791-2799.	14.6	14
26	Dynamics of Photoexcited Small Polarons in Transition-Metal Oxides. Journal of Physical Chemistry Letters, 2021, 12, 2191-2198.	4.6	41
27	First-Principles Prediction of Two-Dimensional B₃C₂P₃ and B₂C₄P₂: Structural Stability, Fundamental Properties, and Renewable Energy Applications. Journal of Physical Chemistry Letters, 2021, 12, 3436-3442.	4.6	34
28	Concentric Approximation for Fast and Accurate Numerical Evaluation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2021, 12, 3082-3089.	4.6	41
29	Why Hybrid Tin-Based Perovskites Simultaneously Improve the Structural Stability and Charge Carriersâ€™ Lifetime: Ab Initio Quantum Dynamics. ACS Applied Materials & Interfaces, 2021, 13, 16567-16575.	8.0	10
30	Common Defects Accelerate Charge Separation and Reduce Recombination in CNT/Molecule Composites: Atomistic Quantum Dynamics. Journal of the American Chemical Society, 2021, 143, 6649-6656.	13.7	35
31	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
32	Strong Modulation of Band Gap, Carrier Mobility and Lifetime in Two-Dimensional Black Phosphorene through Acoustic Phonon Excitation. Journal of Physical Chemistry Letters, 2021, 12, 3960-3967.	4.6	30
33	Band alignment and defects influence the electronâ€“phonon heat transport mechanisms across metal interfaces. Applied Physics Letters, 2021, 118, .	3.3	8
34	Interpolating Nonadiabatic Molecular Dynamics Hamiltonian with Artificial Neural Networks. Journal of Physical Chemistry Letters, 2021, 12, 6070-6077.	4.6	29
35	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. Journal of the American Chemical Society, 2021, 143, 9982-9990.	13.7	52
36	Mixed Metals Slow Down Nonradiative Recombination in Saddle-Shaped Porphyrin Nanorings: A Time-Domain Atomistic Simulation. Journal of Physical Chemistry C, 2021, 125, 16620-16628.	3.1	7

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37	Discovery of a Wurtzite-like Cu₂FeSnSe₄ Semiconductor Nanocrystal Polymorph and Implications for Related CuFeSe₂ Materials. ACS Nano, 2021, 15, 13463-13474.	14.6	10
38	Common Defects Accelerate Charge Carrier Recombination in CsSnI₃ without Creating Mid-Gap States. Journal of Physical Chemistry Letters, 2021, 12, 8699-8705.	4.6	31
39	Facile Removal of Bulk Oxygen Vacancy Defects in Metal Oxides Driven by Hydrogen-Dopant Evaporation. Journal of Physical Chemistry Letters, 2021, 12, 9579-9583.	4.6	1
40	Analytic Model of Nonequilibrium Charge Transport in Disordered Organic Semiconductors with Combined Energy and Off-Diagonal Disorder. Journal of Physical Chemistry C, 2021, 125, 20230-20240.	3.1	1
41	Dependence between Structural and Electronic Properties of CsPbI₃: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 8672-8678.	4.6	26
42	Excited-State Properties of Defected Halide Perovskite Quantum Dots: Insights from Computation. Journal of Physical Chemistry Letters, 2021, 12, 1005-1011.	4.6	15
43	Point Defects in Two-Dimensional Î³-Phosphorus Carbide. Journal of Physical Chemistry Letters, 2021, 12, 620-626.	4.6	21
44	Identifying and Passivating Killer Defects in Pb-Free Double Cs₂AgBiBr₆ Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 10581-10588.	4.6	17
45	Generating Shear Flows without Moving Parts by Thermo-osmosis in Heterogeneous Nanochannels. Journal of Physical Chemistry Letters, 2021, 12, 10099-10105.	4.6	7
46	Nonadiabatic molecular dynamics analysis of hybrid Dionâ€“Jacobson 2D leads iodide perovskites. Applied Physics Letters, 2021, 119, .	3.3	9
47	Modeling Non-adiabatic Dynamics in Nanoscale and Condensed Matter Systems. Accounts of Chemical Research, 2021, 54, 4239-4249.	15.6	46
48	Excited-State Dynamics in Metal Halide Perovskites: A Theoretical Perspective. , 2021, , 1-54.		0
49	Influence of intrinsic defects on the structure and dynamics of the mixed Pbâ€“Sn perovskite: first-principles DFT and NAMD simulations. Journal of Materials Chemistry A, 2021, 10, 234-244.	10.3	11
50	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in Cu₂ZnSnS₄Photoabsorbers. ACS Applied Materials & Interfaces, 2021, 13, 61365-61373.	8.0	11
51	Significance of the Chemical Environment of an Element in Nonadiabatic Molecular Dynamics: Feature Selection and Dimensionality Reduction with Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 12026-12032.	4.6	11
52	Electronâ€“phonon coupling and related transport properties of metals and intermetallic alloys from first principles. Materials Today Physics, 2020, 12, 100175.	6.0	23
53	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
54	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. Angewandte Chemie, 2020, 132, 4714-4720.	2.0	18

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55	Edge Influence on Charge Carrier Localization and Lifetime in CH₃NH₃PbBr₃ Perovskite: Ab Initio Quantum Dynamics Simulation. Journal of Physical Chemistry Letters, 2020, 11, 9100-9109.	4.6	39
56	Protecting hot carriers by tuning hybrid perovskite structures with alkali cations. Science Advances, 2020, 6, .	10.3	54
57	Net Unidirectional Fluid Transport in Locally Heated Nanochannel by Thermo-osmosis. Nano Letters, 2020, 20, 8965-8971.	9.1	23
58	Accurate Computation of Nonadiabatic Coupling with Projector Augmented-Wave Pseudopotentials. Journal of Physical Chemistry Letters, 2020, 11, 10073-10080.	4.6	65
59	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. ACS Energy Letters, 2020, 5, 3813-3820.	17.4	47
60	Quantum dynamics origin of high photocatalytic activity of mixed-phase anatase/rutile TiO2. Journal of Chemical Physics, 2020, 153, 044706.	3.0	26
61	Photoinduced Dynamics of Charge Carriers in Metal Halide Perovskites from an Atomistic Perspective. Journal of Physical Chemistry Letters, 2020, 11, 7066-7082.	4.6	41
62	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
63	Ab initio quantum dynamics of charge carriers in graphitic carbon nitride nanosheets. Journal of Chemical Physics, 2020, 153, 054701.	3.0	27
64	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
65	Advancing Physical Chemistry with Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 9656-9658.	4.6	48
66	Influence of tungsten doping on nonradiative electronâ€“hole recombination in monolayer MoSe2 with Se vacancies. Journal of Chemical Physics, 2020, 153, 154701.	3.0	8
67	Thermal smearing in DFT calculations: How small is really small? A case of La and Lu atoms adsorbed on graphene. Materials Today Communications, 2020, 25, 101595.	1.9	18
68	Combining Lindblad Master Equation and Surface Hopping to Evolve Distributions of Quantum Particles. Journal of Physical Chemistry B, 2020, 124, 4326-4337.	2.6	13
69	Structural Deformation Controls Charge Losses in MAPbI₃: Unsupervised Machine Learning of Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2020, 5, 1930-1938.	17.4	55
70	MAI Termination Favors Efficient Hole Extraction and Slow Charge Recombination at the MAPbI₃/CuSCN Heterojunction. Journal of Physical Chemistry Letters, 2020, 11, 4481-4489.	4.6	22
71	Anti-correlation between Band gap and Carrier Lifetime in Lead Halide Perovskites under Compression Rationalized by Ab Initio Quantum Dynamics. Chemistry of Materials, 2020, 32, 4707-4715.	6.7	36
72	Atomic fluctuations in electronic materials revealed by dephasing. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11940-11946.	7.1	27

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73	Iodine and Sulfur Vacancy Cooperation Promotes Ultrafast Charge Extraction at MAPbI₃/MoS₂ Interface. ACS Energy Letters, 2020, 5, 1346-1354.	17.4	53
74	Sharp-tip enhanced catalytic CO oxidation by atomically dispersed Pt₁/Pt₂on a raised graphene oxide platform. Journal of Materials Chemistry A, 2020, 8, 12485-12494.	10.3	9
75	Low-frequency lattice phonons in halide perovskites explain high defect tolerance toward electron-hole recombination. Science Advances, 2020, 6, eaaw7453.	10.3	182
76	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
77	Pb dimerization greatly accelerates charge losses in MAPbI3: Time-domain ab initio analysis. Journal of Chemical Physics, 2020, 152, 064707.	3.0	12
78	Improved description of hematite surfaces by the SCAN functional. Journal of Chemical Physics, 2020, 152, 024706.	3.0	13
79	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
80	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
81	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
82	Control of Charge Carrier Dynamics in Plasmonic Au Films by TiO_x Substrate Stoichiometry. Journal of Physical Chemistry Letters, 2020, 11, 1419-1427.	4.6	21
83	Soft Lattice and Defect Covalency Rationalize Tolerance of Î²â€CsPbI₃ Perovskite Solar Cells to Native Defects. Angewandte Chemie, 2020, 132, 6497-6503.	2.0	8
84	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
85	Phonon-Suppressed Auger Scattering of Charge Carriers in Defective Two-Dimensional Transition Metal Dichalcogenides. Nano Letters, 2019, 19, 6078-6086.	9.1	43
86	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	2.5	2
87	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	2.6	1
88	Triplet Excitons in Small Helium Clusters. Journal of Physical Chemistry A, 2019, 123, 6113-6122.	2.5	1
89	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	3.1	1
90	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	4.6	2

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91	Anharmonicity Extends Carrier Lifetimes in Lead Halide Perovskites at Elevated Temperatures. Journal of Physical Chemistry Letters, 2019, 10, 6219-6226.	4.6	66
92	Electronâ€“Phonon Scattering Is Much Weaker in Carbon Nanotubes than in Graphene Nanoribbons. Journal of Physical Chemistry Letters, 2019, 10, 7179-7187.	4.6	21
93	Enhanced Activity of C₂N-Supported Single Co Atom Catalyst by Single Atom Promoter. Journal of Physical Chemistry Letters, 2019, 10, 7009-7014.	4.6	35
94	Electronâ€“Phonon Relaxation at Au/Ti Interfaces Is Robust to Alloying: Ab Initio Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry C, 2019, 123, 22842-22850.	3.1	9
95	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
96	Core-dependent properties of copper nanoclusters: valence-pure nanoclusters as NIR TADF emitters and mixed-valence ones as semiconductors. Chemical Science, 2019, 10, 10122-10128.	7.4	42
97	Suppression of Electronâ€“Hole Recombination by Intrinsic Defects in 2D Monoelemental Material. Journal of Physical Chemistry Letters, 2019, 10, 6151-6158.	4.6	62
98	Size-Programmed Synthesis of PbSe Quantum Dots via Secondary Phosphine Chalcogenides. Chemistry of Materials, 2019, 31, 8301-8307.	6.7	9
99	Numerical tests of coherence-corrected surface hopping methods using a donor-bridge-acceptor model system. Journal of Chemical Physics, 2019, 150, 194104.	3.0	17
100	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
101	Ehrenfest and classical path dynamics with decoherence and detailed balance. Journal of Chemical Physics, 2019, 150, 204124.	3.0	40
102	Strong Influence of Oxygen Vacancy Location on Charge Carrier Losses in Reduced TiO₂ Nanoparticles. Journal of Physical Chemistry Letters, 2019, 10, 2676-2683.	4.6	32
103	Thin Ti adhesion layer breaks bottleneck to hot hole relaxation in Au films. Journal of Chemical Physics, 2019, 150, 184701.	3.0	14
104	Coexistence of Different Charge-Transfer Mechanisms in the Hot-Carrier Dynamics of Hybrid Plasmonic Nanomaterials. Nano Letters, 2019, 19, 3187-3193.	9.1	34
105	First-principles determination of the ultrahigh electrical and thermal conductivity in free-electron metals via pressure tuning the electron-phonon coupling factor. Physical Review B, 2019, 99, .	3.2	20
106	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
107	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
108	Catalytic Chemistry Predicted by a Charge Polarization Descriptor: Synergistic O₂ Activation and CO Oxidation by Auâ€“Cu Bimetallic Clusters on TiO₂(101). ACS Applied Materials & Interfaces, 2019, 11, 9629-9640.	8.0	28

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109	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
110	Dependence of electron transfer dynamics on the number of graphene layers in Ï€-stacked 2D materials: insights from ab initio nonadiabatic molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 23198-23208.	2.8	10
111	Strain Controls Charge Carrier Lifetimes in Monolayer WSe₂: Ab Initio Time Domain Analysis. Journal of Physical Chemistry Letters, 2019, 10, 7732-7739.	4.6	36
112	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. Journal of the American Chemical Society, 2019, 141, 20222-20233.	13.7	42
113	JPCL: A Dynamic Journal with a Global Reach. Journal of Physical Chemistry Letters, 2019, 10, 113-114.	4.6	0
114	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
115	Molecular Photophysics under Shock Compression: Ab Initio Nonadiabatic Molecular Dynamics of Rhodamine Dye. Journal of Physical Chemistry C, 2018, 122, 13600-13607.	3.1	4
116	DFT study of the infrared and Raman spectra of photochromic Fulgide;		

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127	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
128	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
129	Persistent Quantum Coherence and Strong Coupling Enable Fast Electron Transfer across the CdS/TiO₂ Interface: A Time-Domain ab Initio Simulation. Journal of Physical Chemistry C, 2018, 122, 25606-25616.	3.1	16
130	Phonon-coupled ultrafast interlayer charge oscillation at van der Waals heterostructure interfaces. Physical Review B, 2018, 97, .	3.2	81
131	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
132	C₂N-supported single metal ion catalysts for HCOOH dehydrogenation. Journal of Materials Chemistry A, 2018, 6, 11105-11112.	10.3	40
133	Hot-Hole Cooling Controls the Initial Ultrafast Relaxation in Methylammonium Lead Iodide Perovskite. Scientific Reports, 2018, 8, 8115.	3.3	32
134	Influence of Encapsulated Water on Luminescence Energy, Line Width, and Lifetime of Carbon Nanotubes: Time Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 4006-4013.	4.6	21
135	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
136	Long Carrier Lifetimes in PbI₂-Rich Perovskites Rationalized by Ab Initio Nonadiabatic Molecular Dynamics. ACS Energy Letters, 2018, 3, 1868-1874.	17.4	54
137	Spinâ€“Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. ACS Energy Letters, 2018, 3, 2159-2166.	17.4	114
138	Superatom Molecular Orbital as an Interfacial Charge Separation State. Journal of Physical Chemistry Letters, 2018, 9, 3485-3490.	4.6	29
139	Real-Time Atomistic Dynamics of Energy Flow in an STM Setup: Revealing the Mechanism of Current-Induced Molecular Emission. Journal of Physical Chemistry Letters, 2018, 9, 3591-3597.	4.6	10
140	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€“Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	5.3	39
141	Ultrafast, asymmetric charge transfer and slow charge recombination in porphyrin/CNT composites demonstrated by time-domain atomistic simulation. Nanoscale, 2018, 10, 12683-12694.	5.6	25
142	Theoretical Investigation of Relaxation Dynamics in Au₃₈(SH)₂₄ Thiolate-Protected Gold Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 16380-16388.	3.1	27
143	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
144	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

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145	Microwave reduction of graphene oxide rationalized by reactive molecular dynamics. Nanoscale, 2017, 9, 4024-4033.	5.6	28
146	Atomistic Analysis of Room Temperature Quantum Coherence in Two-Dimensional CdSe Nanostructures. Nano Letters, 2017, 17, 2389-2396.	9.1	29
147	Two-Dimensional Linear Dichroism Spectroscopy for Identifying Protein Orientation and Secondary Structure Composition. Journal of Physical Chemistry Letters, 2017, 8, 1031-1037.	4.6	5
148	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
149	Cooperative enhancement of the nonlinear optical response in conjugated energetic materials: A TD-DFT study. Journal of Chemical Physics, 2017, 146, 114308.	3.0	13
150	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
151	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
152	Weak Donorâ€“Acceptor Interaction and Interface Polarization Define Photoexcitation Dynamics in the MoS₂/TiO₂ Composite: Time-Domain Ab Initio Simulation. Nano Letters, 2017, 17, 4038-4046.	9.1	45
153	Quantum Dynamics of Photogenerated Charge Carriers in Hybrid Perovskites: Dopants, Grain Boundaries, Electric Order, and Other Realistic Aspects. ACS Energy Letters, 2017, 2, 1588-1597.	17.4	31
154	Imidazolium Ionic Liquid Mediates Black Phosphorus Exfoliation while Preventing Phosphorene Decomposition. ACS Nano, 2017, 11, 6459-6466.	14.6	43
155	Nonadiabatic charge dynamics in novel solar cell materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1305.	14.6	71
156	Analytic Modeling of Field Dependence of Charge Mobility and Applicability of the Concept of the Effective Transport Level to an Organic Dipole Glass. Journal of Physical Chemistry C, 2017, 121, 7776-7781.	3.1	8
157	Time-Domain ab Initio Modeling of Electronâ€“Phonon Relaxation in High-Temperature Cuprate Superconductors. Journal of Physical Chemistry Letters, 2017, 8, 193-198.	4.6	20
158	The JPCL New Yearâ€™s Editorial. Journal of Physical Chemistry Letters, 2017, 8, 41-41.	4.6	0
159	Exfoliation of Graphene in Ionic Liquids: Pyridinium versus Pyrrolidinium. Journal of Physical Chemistry C, 2017, 121, 911-917.	3.1	30
160	Perspective Collections in the Limelight. Journal of Physical Chemistry Letters, 2017, 8, 5239-5239.	4.6	0
161	In the Limelight. Journal of Physical Chemistry Letters, 2017, 8, 3925-3925.	4.6	0
162	Phonon-Assisted Ultrafast Charge Transfer at van der Waals Heterostructure Interface. Nano Letters, 2017, 17, 6435-6442.	9.1	204

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163	Temperature Dependence of Electronâ€“Phonon Interactions in Gold Films Rationalized by Time-Domain Ab Initio Analysis. Journal of Physical Chemistry C, 2017, 121, 17488-17497.	3.1	21
164	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
165	Optoelectronic Properties of Semiconductor Quantum Dot Solids for Photovoltaic Applications. Journal of Physical Chemistry Letters, 2017, 8, 4129-4139.	4.6	71
166	In the Limelight. Journal of Physical Chemistry Letters, 2017, 8, 3718-3719.	4.6	0
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