

# Run Long

## List of Publications by Year in descending order

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190  
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192  
docs citations

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times ranked

8829  
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficient passivation of DY center in CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> by chlorine: Quantum molecular dynamics. Nano Research, 2022, 15, 2112-2122.	5.8	28
2	Bidirectional Light-Driven Ion Transport through Porphyrin Metal-Organic Framework-Based van der Waals Heterostructures via pH-Induced Band Alignment Inversion. CCS Chemistry, 2022, 4, 3329-3341.	4.6	13
3	Stretchable MoS <sub>2</sub> Artificial Photoreceptors for E-Skin. Advanced Functional Materials, 2022, 32, 2107524.	7.8	24
4	Accelerating pH-universal hydrogen-evolving activity of a hierarchical hybrid of cobalt and dinickel phosphides by interfacial chemical bonds. Materials Today Physics, 2022, 22, 100589.	2.9	20
5	Dual Passivation of Point Defects at Perovskite Grain Boundaries with Ammonium Salts Greatly Inhibits Nonradiative Charge Recombination. Journal of Physical Chemistry Letters, 2022, 13, 954-961.	2.1	10
6	Substitutional alkaline earth metals delay nonradiative charge recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite: A time-domain study. Journal of Chemical Physics, 2022, 156, 014702.	1.2	2
7	Large-Area Printing of Ferroelectric Surface and Super-Domain for Solar Water Splitting. Advanced Functional Materials, 2022, 32, .	7.8	17
8	The twist angle has weak influence on charge separation and strong influence on recombination in the MoS <sub>2</sub> /WS <sub>2</sub> bilayer: <i>ab initio</i> quantum dynamics. Journal of Materials Chemistry A, 2022, 10, 8324-8333.	5.2	30
9	Correlated organic-inorganic motion enhances stability and charge carrier lifetime in mixed halide perovskites. Nanoscale, 2022, 14, 4644-4653.	2.8	18
10	Electric Field Effects on Photoelectrochemical Water Splitting: Perspectives and Outlook. Energies, 2022, 15, 1553.	1.6	2
11	N-doped MoS <sub>2</sub> via assembly transfer on an elastomeric substrate for high-photoresponsivity, air-stable and stretchable photodetector. Nano Research, 2022, 15, 9866-9874.	5.8	8
12	Collective Motion Improves the Stability and Charge Carrier Lifetime of Metal Halide Perovskites: A Phonon-Resolved Nonadiabatic Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2022, 13, 3016-3022.	2.1	12
13	Improving Lattice Rigidity and Charge Carrier Lifetime by Engineering Spacer Cation of Ruddlesden-Popper Perovskites: A Time-Domain <i>Ab Initio</i> Study. Journal of Physical Chemistry Letters, 2022, 13, 2718-2724.	2.1	11
14	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.	6.6	29
15	Self-Diffusion of Individual Adsorbed Water Molecules at Rutile (110) and Anatase (101) TiO <sub>2</sub> Interfaces from Molecular Dynamics. Crystals, 2022, 12, 398.	1.0	2
16	Chemical passivation of methylammonium fragments eliminates traps, extends charge lifetimes, and restores structural stability of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite. Nano Research, 2022, 15, 4765-4772.	5.8	12
17	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO <sub>2</sub> (110) Surface. JACS Au, 2022, 2, 234-245.	3.6	22
18	Unveiling the Valence State of Interstitial Bromine on Charge Carrier Lifetime in CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> by Quantum Dynamics Simulation. Journal of Physical Chemistry Letters, 2022, 13, 4193-4199.	2.1	2

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19	Understanding Competitive Photo-Induced Molecular Oxygen Dissociation and Desorption Dynamics atop a Reduced Rutile TiO <sub>2</sub> (110) Surface: A Time-Domain Ab Initio Study. ACS Catalysis, 2022, 12, 6702-6711.	5.5	13
20	Depleted Oxygen Defect State Enhancing Tungsten Trioxide Photocatalysis: A Quantum Dynamics Perspective. Journal of Physical Chemistry Letters, 2022, 13, 5571-5580.	2.1	15
21	Synergistic effect of atomic layer deposition-assisted cocatalyst and crystal facet engineering in SnS <sub>2</sub> nanosheet for solar water oxidation. Science Bulletin, 2022, 67, 1562-1571.	4.3	14
22	Photoinduced small electron polarons generation and recombination in hematite. Npj Computational Materials, 2022, 8, .	3.5	10
23	Bidentate Lewis bases are preferred for passivation of MAPbI <sub>3</sub> surfaces: A time-domain ab initio analysis. Nano Energy, 2021, 79, 105491.	8.2	33
24	Weak Distance Dependence of Hot-Electron-Transfer Rates at the Interface between Monolayer MoS <sub>2</sub> and Gold. ACS Nano, 2021, 15, 819-828.	7.3	27
25	Doping-Induced Charge Localization Suppresses Electron-Hole Recombination in Copper Zinc Tin Sulfide: Quantum Dynamics Combined with Deep Neural Networks Analysis. Journal of Physical Chemistry Letters, 2021, 12, 835-842.	2.1	15
26	Phonon-Mediated Interlayer Charge Separation and Recombination in a MoSe <sub>2</sub> /WSe <sub>2</sub> Heterostructure. Nano Letters, 2021, 21, 2165-2173.	4.5	46
27	Preventing Superoxide Generation on Molecule-Protected CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskite: A Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2021, 12, 1664-1670.	2.1	13
28	Rapid Charge Separation Boosts Solar Hydrogen Generation at the Graphene-MoS <sub>2</sub> Junction: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2021, 12, 2763-2769.	2.1	16
29	Harnessing Ionic Power from Equilibrium Electrolyte Solution via Photoinduced Active Ion Transport through vanâ€derâ€Waalâ€Like Heterostructures. Advanced Materials, 2021, 33, e2007529.	11.1	37
30	High-performance large-area quasi-2D perovskite light-emitting diodes. Nature Communications, 2021, 12, 2207.	5.8	173
31	Water Splitting with a Single-Atom Cu/TiO <sub>2</sub> Photocatalyst: Atomistic Origin of High Efficiency and Proposed Enhancement by Spin Selection. JACS, 2021, 143, 550-559.	3.6	58
32	Controlling Charge Carrier Trapping and Recombination in BiVO <sub>4</sub> with the Oxygen Vacancy Oxidation State. Journal of Physical Chemistry Letters, 2021, 12, 3514-3521.	2.1	33
33	Marked Passivation Effect of Naphthalene-1,8-diCarboximides in High-Performance Perovskite Solar Cells. Advanced Materials, 2021, 33, e2008405.	11.1	116
34	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. Journal of the American Chemical Society, 2021, 143, 9982-9990.	6.6	52
35	Thermal-Driven Dynamic Shape Change of Bimetallic Nanoparticles Extends Hot Electron Lifetime of Pt/MoS <sub>2</sub> Catalysts. Journal of Physical Chemistry Letters, 2021, 12, 7173-7179.	2.1	8
36	Paraffin-Enabled Compressive Folding of Two-Dimensional Materials with Controllable Broadening of the Electronic Band Gap. ACS Applied Materials & Interfaces, 2021, 13, 40922-40931.	4.0	8

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37	Photoinduced Anomalous Electron Transfer Dynamics at a Lateral MoS <sub>2</sub> –Graphene Covalent Junction. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 7553-7559.	2.1	12
38	Benign Effects of Twin Boundaries on Charge Carrier Lifetime in Metal Halide Perovskites by a Time-Domain Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8575-8582.	2.1	13
39	Atomic layer deposition triggered Fe-In-S cluster and gradient energy band in ZnInS photoanode for improved oxygen evolution reaction. <i>Nature Communications</i> , 2021, 12, 5247.	5.8	36
40	Density Functional Theory Half-Electron Self-Energy Correction for Fast and Accurate Nonadiabatic Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10886-10892.	2.1	10
41	Charge-Compensated Doping Extends Carrier Lifetimes in SrTiO <sub>3</sub> by Passivating Oxygen Vacancy Defects. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12040-12047.	2.1	20
42	Ferroelastic domains drive charge separation and suppress electron–hole recombination in all-inorganic halide perovskites: time-domain <i>ab initio</i> analysis. <i>Nanoscale Horizons</i> , 2020, 5, 683-690.	4.1	20
43	Covalent Functionalized Black Phosphorus Greatly Inhibits Nonradiative Charge Recombination: A Time Domain <i>Ab Initio</i> Study. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 478-484.	2.1	22
44	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4684-4690.	7.2	78
45	Extending Carrier Lifetimes in Lead Halide Perovskites with Alkali Metals by Passivating and Eliminating Halide Interstitial Defects. <i>Angewandte Chemie</i> , 2020, 132, 4714-4720.	1.6	18
46	Weak temperature-dependent hole injection and electron–hole recombination at the CH <sub>3</sub> NH <sub>3</sub> Pb <sub>3</sub> /NiO heterojunction: a time-domain <i>ab initio</i> study. <i>Journal of Materials Chemistry A</i> , 2020, 8, 607-615.	5.2	16
47	Design of a Z-scheme g-C <sub>3</sub> N <sub>4</sub> /CQDs/CdIn <sub>2</sub> S <sub>4</sub> composite for efficient visible-light-driven photocatalytic degradation of ibuprofen. <i>Environmental Pollution</i> , 2020, 259, 113770.	3.7	50
48	Edge Influence on Charge Carrier Localization and Lifetime in CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> Perovskite: <i>Ab Initio</i> Quantum Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9100-9109.	2.1	39
49	Isotopic Exchange Extends Charge Carrier Lifetime in Metal Lead Perovskites by Quantum Dynamics Simulations. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10298-10305.	2.1	11
50	Unraveling the quantum dynamics origin of high photocatalytic activity in nitrogen-doped anatase TiO <sub>2</sub> : time-domain <i>ab initio</i> analysis. <i>Journal of Materials Chemistry A</i> , 2020, 8, 25235-25244.	5.2	19
51	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. <i>ACS Energy Letters</i> , 2020, 5, 3813-3820.	8.8	47
52	Quantum dynamics origin of high photocatalytic activity of mixed-phase anatase/rutile TiO <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2020, 153, 044706.	1.2	26
53	Photoinduced Dynamics of Charge Carriers in Metal Halide Perovskites from an Atomistic Perspective. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7066-7082.	2.1	41
54	Why Oxygen Increases Carrier Lifetimes but Accelerates Degradation of CH <sub>3</sub> NH <sub>3</sub> Pb <sub>3</sub> under Light Irradiation: Time-Domain <i>Ab Initio</i> Analysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 14664-14673.	6.6	64

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55	Influence of tungsten doping on nonradiative electron-hole recombination in monolayer MoSe <sub>2</sub> with Se vacancies. <i>Journal of Chemical Physics</i> , 2020, 153, 154701.	1.2	8
56	Oxidation Notably Accelerates Nonradiative Electron-Hole Recombination in MoS <sub>2</sub> by Different Mechanisms: Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4086-4092.	2.1	17
57	MAI Termination Favors Efficient Hole Extraction and Slow Charge Recombination at the MAPbI <sub>3</sub> /CuSCN Heterojunction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4481-4489.	2.1	22
58	Substrate-free flexible thin film solar cells by graphene-mediated peel-off technology. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 10279-10287.	1.1	1
59	Two-Dimensional Perovskite Capping Layer Simultaneously Improves the Charge Carriers' Lifetime and Stability of MAPbI <sub>3</sub> Perovskite: A Time-Domain Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5100-5107.	2.1	9
60	Covalently Connected Nb <sub>4</sub> N <sub>5</sub> O <sub>2</sub> MoS <sub>2</sub> Heterocatalysts with Desired Electron Density to Boost Hydrogen Evolution. <i>ACS Nano</i> , 2020, 14, 4925-4937.	7.3	50
61	Rapid Decoherence Induced by Light Expansion Suppresses Charge Recombination in Mixed Cation Perovskites: Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1601-1608.	2.1	19
62	Pb dimerization greatly accelerates charge losses in MAPbI <sub>3</sub> : Time-domain ab initio analysis. <i>Journal of Chemical Physics</i> , 2020, 152, 064707.	1.2	12
63	Direct Growth of Continuous and Uniform MoS <sub>2</sub> Film on SiO <sub>2</sub> /Si Substrate Catalyzed by Sodium Sulfate. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1570-1577.	2.1	15
64	Reduced-dimensional perovskite photovoltaics with homogeneous energy landscape. <i>Nature Communications</i> , 2020, 11, 1672.	5.8	191
65	The Interplay Between Lead Vacancy and Water Rationalizes the Puzzle of Charge Carrier Lifetimes in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> : Time-Domain Ab Initio Analysis. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 13347-13353.	7.2	24
66	The Interplay Between Lead Vacancy and Water Rationalizes the Puzzle of Charge Carrier Lifetimes in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> : Time-Domain Ab Initio Analysis. <i>Angewandte Chemie</i> , 2020, 132, 13449-13455.	1.6	0
67	Charge localization control of electron-hole recombination in multilayer two-dimensional Dion-Jacobson hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 2020, 8, 9168-9176.	5.2	38
68	Charge Localization Induced by Nanopore Defects in Monolayer Black Phosphorus for Suppressing Nonradiative Electron-Hole Recombination through Time-Domain Simulation. <i>Wuli Huaxue Xuebao/Acta Physico-Chimica Sinica</i> , 2020, .	2.2	6
69	Charge localization induced by reorientation of FA cations greatly suppresses nonradiative electron-hole recombination in FAPbI <sub>3</sub> perovskites: A time-domain Ab Initio study. <i>Chinese Journal of Chemical Physics</i> , 2020, 33, 642-648.	0.6	1
70	Ni/Fe Codoped In <sub>2</sub> S <sub>3</sub> Nanosheet Arrays Boost Photoelectrochemical Performance of Planar Si Photocathodes. <i>Advanced Energy Materials</i> , 2019, 9, 1902135.	10.2	47
71	Anomalous Temperature-Dependent Charge Recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskite: Key Roles of Charge Localization and Thermal Effect. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 32069-32075.	4.0	22
72	Unravelling the Effects of Pressure-Induced Suppressed Electron-Hole Recombination in CsPbBr <sub>3</sub> Perovskite: Time-Domain ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4354-4361.	2.1	19

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73	Efficient and Stable Inverted Perovskite Solar Cells Incorporating Secondary Amines. <i>Advanced Materials</i> , 2019, 31, e1903559.	11.1	128
74	A Plasma-Triggered O-S Bond and P-N Junction Near the Surface of a SnS <sub>2</sub> Nanosheet Array to Enable Efficient Solar Water Oxidation. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16668-16675.	7.2	42
75	Site Cation Engineering for Highly Efficient MAPbI <sub>3</sub> Single-Crystal X-ray Detector. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17834-17842.	7.2	174
76	Hole Localization Inhibits Charge Recombination in Tin-Lead Mixed Perovskites: Time-Domain ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6604-6612.	2.1	21
77	Perovskite Solar Cells: Efficient and Stable Inverted Perovskite Solar Cells Incorporating Secondary Amines ( <i>Adv. Mater.</i> 46/2019). <i>Advanced Materials</i> , 2019, 31, 1970330.	11.1	1
78	Ferroelectric Polarization Suppresses Nonradiative Electron-Hole Recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskites: A Time-Domain ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7237-7244.	2.1	17
79	Site Cation Engineering for Highly Efficient MAPbI <sub>3</sub> Single-Crystal X-ray Detector. <i>Angewandte Chemie</i> , 2019, 131, 17998-18006.	1.6	15
80	A Plasma-Triggered O-S Bond and P-N Junction Near the Surface of a SnS <sub>2</sub> Nanosheet Array to Enable Efficient Solar Water Oxidation. <i>Angewandte Chemie</i> , 2019, 131, 16821-16828.	1.6	11
81	An <i>in situ</i> constructed topological rich vacancy-defect nitrogen-doped nanocarbon as a highly-effective metal-free oxygen catalyst for Li-O <sub>2</sub> batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 21918-21926.	5.2	18
82	Ultrafast Charge Separation and Recombination across a Molecule/CsPbBr <sub>3</sub> Quantum Dot Interface from First-Principles Nonadiabatic Molecular Dynamics Simulation. <i>Journal of Physical Chemistry C</i> , 2019, 123, 23800-23806.	1.5	8
83	Exciton Dissociation and Suppressed Charge Recombination at 2D Perovskite Edges: Key Roles of Unsaturated Halide Bonds and Thermal Disorder. <i>Journal of the American Chemical Society</i> , 2019, 141, 15557-15566.	6.6	98
84	Surface Pb-Dimer Passivated by Molecule Oxygen Notably Suppresses Charge Recombination in CsPbBr <sub>3</sub> Perovskites: Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5499-5506.	2.1	22
85	Unravelling the effects of oxidation state of interstitial iodine and oxygen passivation on charge trapping and recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> perovskite: a time-domain <i>ab initio</i> study. <i>Chemical Science</i> , 2019, 10, 10079-10088.	3.7	44
86	Mixed Cs and FA Cations Slow Electron-Hole Recombination in FAPbI <sub>3</sub> Perovskites by Time-Domain Ab Initio Study: Lattice Contraction versus Octahedral Tilting. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 672-678.	2.1	29
87	Influence of Defects on Excited-State Dynamics in Lead Halide Perovskites: Time-Domain ab Initio Studies. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3788-3804.	2.1	66
88	Doping-Induced Rapid Decoherence Suppresses Charge Recombination in Mono/Divalent Cation Mixed Perovskites from Nonadiabatic Molecular Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3433-3439.	2.1	24
89	Hydrogen Passivated Silicon Grain Boundaries Greatly Reduce Charge Recombination for Improved Silicon/Perovskite Tandem Solar Cell Performance: Time Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2445-2452.	2.1	14
90	Doping-Induced Amorphization, Vacancy, and Gradient Energy Band in SnS <sub>2</sub> Nanosheet Arrays for Improved Photoelectrochemical Water Splitting. <i>Angewandte Chemie</i> , 2019, 131, 6833-6837.	1.6	23

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91	Doping-Induced Amorphization, Vacancy, and Gradient Energy Band in SnS <sub>2</sub> Nanosheet Arrays for Improved Photoelectrochemical Water Splitting. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6761-6765.	7.2	125
92	Superoxide/Peroxide Chemistry Extends Charge Carriers' Lifetime but Undermines Chemical Stability of CH <sub>3</sub> NH <sub>3</sub> Pb <sub>3</sub> Exposed to Oxygen: Time-Domain <i>ab Initio</i> Analysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 5798-5807.	6.6	102
93	Symmetry Breaking at MAPb <sub>3</sub> Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain <i>ab Initio</i> Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1617-1623.	2.1	65
94	Chlorine Passivation of Grain Boundary Suppresses Electron-Hole Recombination in CsPbBr <sub>3</sub> Perovskite by Nonadiabatic Molecular Dynamics Simulation. <i>ACS Applied Energy Materials</i> , 2019, 2, 3419-3426.	2.5	32
95	Interfacial Engineering Determines Band Alignment and Steers Charge Separation and Recombination at an Inorganic Perovskite Quantum Dot/WS <sub>2</sub> Junction: A Time Domain <i>ab Initio</i> Study. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1234-1241.	2.1	25
96	Strain Controls Charge Carrier Lifetimes in Monolayer WSe <sub>2</sub> : <i>ab Initio</i> Time Domain Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7732-7739.	2.1	36
97	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. <i>Journal of the American Chemical Society</i> , 2019, 141, 20222-20233.	6.6	42
98	Lewis Base Passivation of Hybrid Halide Perovskites Slows Electron-Hole Recombination: Time-Domain <i>ab Initio</i> Analysis. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1164-1171.	2.1	90
99	Significant enhancement of the performance of hydrogen evolution reaction through shape-controlled synthesis of hierarchical dendrite-like platinum. <i>Journal of Materials Chemistry A</i> , 2018, 6, 8068-8077.	5.2	46
100	Plasmon-Mediated Electron Injection from Au Nanorods into MoS <sub>2</sub> : Traditional versus Photoexcitation Mechanism. <i>CheM</i> , 2018, 4, 1112-1127.	5.8	71
101	Halide Composition Controls Electron-Hole Recombination in Cesium-Lead Halide Perovskite Quantum Dots: A Time Domain <i>ab Initio</i> Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1872-1879.	2.1	103
102	Nonadiabatic Molecular Dynamics Simulation of Charge Separation and Recombination at a WS <sub>2</sub> /QD Heterojunction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7041-7050.	1.5	16
103	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain <i>ab Initio</i> Analysis. <i>Nano Letters</i> , 2018, 18, 2459-2466.	4.5	114
104	Dopant Control of Electron-Hole Recombination in Cesium-Titanium Halide Double Perovskite by Time Domain <i>ab Initio</i> Simulation: Codoping Supersedes Monodoping. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6907-6914.	2.1	24
105	Layer-Coupled States Facilitate Ultrafast Charge Transfer in a Transition Metal Dichalcogenide Trilayer Heterostructure. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5970-5978.	2.1	16
106	Grain Boundary Facilitates Photocatalytic Reaction in Rutile TiO <sub>2</sub> Despite Fast Charge Recombination: A Time-Domain <i>ab Initio</i> Analysis. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5884-5889.	2.1	27
107	Lead Vacancy Can Explain the Suppressed Nonradiative Electron-Hole Recombination in FAPb <sub>3</sub> Perovskite under Iodine-Rich Conditions: A Time-Domain <i>ab Initio</i> Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6489-6495.	2.1	29
108	Photocarrier dynamics in monolayer phosphorene and bulk black phosphorus. <i>Nanoscale</i> , 2018, 10, 11307-11313.	2.8	29

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109	Why Chemical Vapor Deposition Grown MoS <sub>2</sub> Samples Outperform Physical Vapor Deposition Samples: Time-Domain ab Initio Analysis. Nano Letters, 2018, 18, 4008-4014.	4.5	94
110	Photoinduced Localized Hole Delays Nonradiative Electron-Hole Recombination in Cesium-Lead Halide Perovskites: A Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 3021-3028.	2.1	22
111	Grain Boundaries Are Benign and Suppress Nonradiative Electron-Hole Recombination in Monolayer Black Phosphorus: A Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2018, 9, 3856-3862.	2.1	54
112	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.	2.1	21
113	Reductive Transformation of Layered-Double-Hydroxide Nanosheets to Fe-Based Heterostructures for Efficient Visible-Light Photocatalytic Hydrogenation of CO. Advanced Materials, 2018, 30, e1803127.	11.1	100
114	Increased Lattice Stiffness Suppresses Nonradiative Charge Recombination in MAPbI <sub>3</sub> Doped with Larger Cations: Time-Domain Ab Initio Analysis. ACS Energy Letters, 2018, 3, 2070-2076.	8.8	68
115	Unravelling the Effects of A-Site Cations on Nonradiative Electron-Hole Recombination in Lead Bromide Perovskites: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 4834-4840.	2.1	24
116	Donor-Acceptor Interaction Determines the Mechanism of Photoinduced Electron Injection from Graphene Quantum Dots into TiO <sub>2</sub> : I $\pi$ -Stacking Supersedes Covalent Bonding. Journal of the American Chemical Society, 2017, 139, 2619-2629.	6.6	132
117	Strong Interaction at the Perovskite/TiO <sub>2</sub> Interface Facilitates Ultrafast Photoinduced Charge Separation: A Nonadiabatic Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 3797-3806.	1.5	69
118	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.	6.6	132
119	Weak Donor-Acceptor Interaction and Interface Polarization Define Photoexcitation Dynamics in the MoS <sub>2</sub> /TiO <sub>2</sub> Composite: Time-Domain Ab Initio Simulation. Nano Letters, 2017, 17, 4038-4046.	4.5	45
120	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.	8.8	31
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