

# Run Long

## List of Publications by Year in descending order

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190  
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docs citations

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#	ARTICLE	IF	CITATIONS
1	Unravelling the Effects of Grain Boundary and Chemical Doping on Electron–Hole Recombination in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Perovskite by Time-Domain Atomistic Simulation. <i>Journal of the American Chemical Society</i> , 2016, 138, 3884-3890.	13.7	333
2	Ultrafast Carrier Thermalization and Cooling Dynamics in Few-Layer MoS <sub>2</sub> . <i>ACS Nano</i> , 2014, 8, 10931-10940.	14.6	236
3	Photo-induced Charge Separation across the Graphene–TiO <sub>2</sub> Interface Is Faster than Energy Losses: A Time-Domain <i>ab Initio</i> Analysis. <i>Journal of the American Chemical Society</i> , 2012, 134, 14238-14248.	13.7	226
4	Quantum Coherence Facilitates Efficient Charge Separation at a MoS <sub>2</sub> /MoSe <sub>2</sub> van der Waals Junction. <i>Nano Letters</i> , 2016, 16, 1996-2003.	9.1	225
5	Instantaneous Generation of Charge-Separated State on TiO <sub>2</sub> Surface Sensitized with Plasmonic Nanoparticles. <i>Journal of the American Chemical Society</i> , 2014, 136, 4343-4354.	13.7	221
6	Reduced-dimensional perovskite photovoltaics with homogeneous energy landscape. <i>Nature Communications</i> , 2020, 11, 1672.	12.8	191
7	A–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.	13.8	174
8	High-performance large-area quasi-2D perovskite light-emitting diodes. <i>Nature Communications</i> , 2021, 12, 2207.	12.8	173
9	Moderate Humidity Delays Electron–Hole Recombination in Hybrid Organic–Inorganic Perovskites: Time-Domain <i>Ab Initio</i> Simulations Rationalize Experiments. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3215-3222.	4.6	139
10	Sulfur Adatom and Vacancy Accelerate Charge Recombination in MoS <sub>2</sub> but by Different Mechanisms: Time-Domain <i>Ab Initio</i> Analysis. <i>Nano Letters</i> , 2017, 17, 7962-7967.	9.1	136
11	Synergistic Effects on Band Gap-Narrowing in Titania by Codoping from First-Principles Calculations. <i>Chemistry of Materials</i> , 2010, 22, 1616-1623.	6.7	134
12	Donor–Acceptor Interaction Determines the Mechanism of Photoinduced Electron Injection from Graphene Quantum Dots into TiO <sub>2</sub> : I–Stacking Supersedes Covalent Bonding. <i>Journal of the American Chemical Society</i> , 2017, 139, 2619-2629.	13.7	132
13	Control of Charge Carriers Trapping and Relaxation in Hematite by Oxygen Vacancy Charge: <i>Ab Initio</i> Non-adiabatic Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2017, 139, 6707-6717.	13.7	132
14	Efficient and Stable Inverted Perovskite Solar Cells Incorporating Secondary Amines. <i>Advanced Materials</i> , 2019, 31, e1903559.	21.0	128
15	Charge Separation and Recombination in Two-Dimensional MoS <sub>2</sub> /WS <sub>2</sub> : Time-Domain <i>ab Initio</i> Modeling. <i>Chemistry of Materials</i> , 2017, 29, 2466-2473.	6.7	127
16	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.	13.8	125
17	Time-Domain <i>Ab Initio</i> Modeling of Photoinduced Dynamics at Nanoscale Interfaces. <i>Annual Review of Physical Chemistry</i> , 2015, 66, 549-579.	10.8	121
18	<i>Ab Initio</i> Nonadiabatic Molecular Dynamics of the Ultrafast Electron Injection from a PbSe Quantum Dot into the TiO <sub>2</sub> Surface. <i>Journal of the American Chemical Society</i> , 2011, 133, 19240-19249.	13.7	120

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19	Marked Passivation Effect of Naphthalene-1,8-dicarboximides in High-Performance Perovskite Solar Cells. <i>Advanced Materials</i> , 2021, 33, e2008405.	21.0	116
20	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain Ab Initio Analysis. <i>Nano Letters</i> , 2018, 18, 2459-2466.	9.1	114
21	First-principles calculation of nitrogen-tungsten codoping effects on the band structure of anatase-titania. <i>Applied Physics Letters</i> , 2009, 94, .	3.3	113
22	Dopants Control Electron-Hole Recombination at Perovskite-TiO <sub>2</sub> Interfaces: Ab Initio Time-Domain Study. <i>ACS Nano</i> , 2015, 9, 11143-11155.	14.6	108
23	Halide Composition Controls Electron-Hole Recombination in Cesium-Lead Halide Perovskite Quantum Dots: A Time Domain Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1872-1879.	4.6	103
24	Superoxide/Peroxide Chemistry Extends Charge Carriers' Lifetime but Undermines Chemical Stability of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Exposed to Oxygen: Time-Domain Ab Initio Analysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 5798-5807.	13.7	102
25	Reductive Transformation of Layered Double Hydroxide Nanosheets to Fe-Based Heterostructures for Efficient Visible-Light Photocatalytic Hydrogenation of CO. <i>Advanced Materials</i> , 2018, 30, e1803127.	21.0	100
26	Nonradiative Electron-Hole Recombination Rate Is Greatly Reduced by Defects in Monolayer Black Phosphorus: Ab Initio Time Domain Study. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 653-659.	4.6	99
27	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.	13.7	98
28	Band gap engineering of (N,Ta)-codoped TiO <sub>2</sub> : A first-principles calculation. <i>Chemical Physics Letters</i> , 2009, 478, 175-179.	2.6	95
29	Why Chemical Vapor Deposition Grown MoS <sub>2</sub> Samples Outperform Physical Vapor Deposition Samples: Time-Domain Ab Initio Analysis. <i>Nano Letters</i> , 2018, 18, 4008-4014.	9.1	94
30	Lewis Base Passivation of Hybrid Halide Perovskites Slows Electron-Hole Recombination: Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1164-1171.	4.6	90
31	Coherence penalty functional: A simple method for adding decoherence in Ehrenfest dynamics. <i>Journal of Chemical Physics</i> , 2014, 140, 194107.	3.0	86
32	Magnetic properties of first-row element-doped ZnS semiconductors: A density functional theory investigation. <i>Physical Review B</i> , 2009, 80, .	3.2	79
33	Energetic and electronic properties of X- (Si, Ge, Sn, Pb) doped TiO <sub>2</sub> from first-principles. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8165.	2.8	78
34	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.	13.8	78
35	First-principle prediction of half-metallic ferrimagnetism of the Heusler alloys Mn <sub>2</sub> CoZ (Z=Al, Ga, Si). <i>npj Computational Materials</i> , 2020, 6, 1-10.	3.0	75
36	Nonadiabatic charge dynamics in novel solar cell materials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1305.	14.6	71

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37	Plasmon-Mediated Electron Injection from Au Nanorods into MoS <sub>2</sub> : Traditional versus Photoexcitation Mechanism. <i>CheM</i> , 2018, 4, 1112-1127.	11.7	71
38	Interplay between Localized and Free Charge Carriers Can Explain Hot Fluorescence in the CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> Perovskite: Time-Domain Ab Initio Analysis. <i>Journal of the American Chemical Society</i> , 2017, 139, 17327-17333.	13.7	70
39	Strong Interaction at the Perovskite/TiO <sub>2</sub> Interface Facilitates Ultrafast Photoinduced Charge Separation: A Nonadiabatic Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3797-3806.	3.1	69
40	Increased Lattice Stiffness Suppresses Nonradiative Charge Recombination in MAPbI <sub>3</sub> Doped with Larger Cations: Time-Domain Ab Initio Analysis. <i>ACS Energy Letters</i> , 2018, 3, 2070-2076.	17.4	68
41	Asymmetry in the Electron and Hole Transfer at a Polymer-Carbon Nanotube Heterojunction. <i>Nano Letters</i> , 2014, 14, 3335-3341.	9.1	67
42	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.	4.6	66
43	Symmetry Breaking at MAPbI <sub>3</sub> Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1617-1623.	4.6	65
44	Why Oxygen Increases Carrier Lifetimes but Accelerates Degradation of CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> under Light Irradiation: Time-Domain Ab Initio Analysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 14664-14673.	13.7	64
45	Minimizing Electron-Hole Recombination on TiO <sub>2</sub> Sensitized with PbSe Quantum Dots: Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2941-2946.	4.6	63
46	Geometric and Electronic Properties of Sn-Doped TiO <sub>2</sub> from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2009, 113, 650-653.	3.1	62
47	Defects Are Needed for Fast Photo-Induced Electron Transfer from a Nanocrystal to a Molecule: Time-Domain Ab Initio Analysis. <i>Journal of the American Chemical Society</i> , 2013, 135, 18892-18900.	13.7	61
48	Water Splitting with a Single-Atom Cu/TiO <sub>2</sub> Photocatalyst: Atomistic Origin of High Efficiency and Proposed Enhancement by Spin Selection. <i>Jacs Au</i> , 2021, 1, 550-559.	7.9	58
49	First-Principles Calculation of Synergistic (N, P)-Codoping Effects on the Visible-Light Photocatalytic Activity of Anatase TiO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2010, 114, 11984-11990.	3.1	55
50	Electronic Structure of Semiconducting and Metallic Tubes in TiO <sub>2</sub> /Carbon Nanotube Heterojunctions: Density Functional Theory Calculations. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1340-1346.	4.6	55
51	Grain Boundaries Are Benign and Suppress Nonradiative Electron-Hole Recombination in Monolayer Black Phosphorus: A Time-Domain Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3856-3862.	4.6	54
52	Structural, Electronic, and Optical Properties of N-doped SnO <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2008, 112, 9861-9864.	3.1	53
53	Tailoring the electronic structure of TiO <sub>2</sub> by cation doping: first-principles calculations. <i>Physical Review B</i> , 2011, 83, 045411.	3.2	52
54	Disparity in Photoexcitation Dynamics between Vertical and Lateral MoS <sub>2</sub> /WSe <sub>2</sub> Heterojunctions: Time-Domain Simulation Emphasizes the Importance of Donor-Acceptor Interaction and Band Alignment. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5771-5778.	4.6	52

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55	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. <i>Journal of the American Chemical Society</i> , 2021, 143, 9982-9990.	13.7	52
56	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.	7.5	50
57	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.	14.6	50
58	Synergistic Effects of Bi/S Codoping on Visible Light-Activated Anatase TiO <sub>2</sub> Photocatalysts from First Principles. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8373-8377.	3.1	49
59	Ultrafast Electron and Hole Relaxation Pathways in Few-Layer MoS <sub>2</sub> . <i>Journal of Physical Chemistry C</i> , 2015, 119, 20698-20708.	3.1	47
60	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.	19.5	47
61	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. <i>ACS Energy Letters</i> , 2020, 5, 3813-3820.	17.4	47
62	Structural and electronic properties of iodine-doped anatase and rutile TiO <sub>2</sub> . <i>Computational Materials Science</i> , 2009, 45, 223-228.	3.0	46
63	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.	10.3	46
64	Phonon-Mediated Interlayer Charge Separation and Recombination in a MoSe <sub>2</sub> /WSe <sub>2</sub> Heterostructure. <i>Nano Letters</i> , 2021, 21, 2165-2173.	9.1	46
65	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. <i>Nano Letters</i> , 2017, 17, 4038-4046.	9.1	45
66	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 ab initio study. <i>Chemical Science</i> , 2019, 10, 10079-10088.	7.4	44
67	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.	13.8	42
68	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. <i>Journal of the American Chemical Society</i> , 2019, 141, 20222-20233.	13.7	42
69	Photoinduced Dynamics of Charge Carriers in Metal Halide Perovskites from an Atomistic Perspective. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7066-7082.	4.6	41
70	Band gap engineering of double-cation-impurity-doped anatase-titania for visible-light photocatalysts: a hybrid density functional theory approach. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13698.	2.8	39
71	Edge Influence on Charge Carrier Localization and Lifetime in CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> Perovskite: Ab Initio Quantum Dynamics Simulation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9100-9109.	4.6	39
72	Electronic structure of cation-codoped TiO <sub>2</sub> for visible-light photocatalyst applications from hybrid density functional theory calculations. <i>Applied Physics Letters</i> , 2011, 98, 142103.	3.3	38

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73	Dimensionality of Nanoscale TiO <sub>2</sub> Determines the Mechanism of Photoinduced Electron Injection from a CdSe Nanoparticle. <i>Nano Letters</i> , 2014, 14, 1790-1796.	9.1	38
74	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.	10.3	38
75	Harnessing Ionic Power from Equilibrium Electrolyte Solution via Photoinduced Active Ion Transport through van der Waals-Like Heterostructures. <i>Advanced Materials</i> , 2021, 33, e2007529.	21.0	37
76	Density functional theory description of the mechanism of ferromagnetism in nitrogen-doped SnO <sub>2</sub> . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009, 374, 319-322.	2.1	36
77	Understanding the Electronic Structures of Graphene Quantum Dot Physisorption and Chemisorption onto the TiO <sub>2</sub> (110) Surface: A First-Principles Calculation. <i>ChemPhysChem</i> , 2013, 14, 579-582.	2.1	36
78	Fullerene Interfaced with a TiO <sub>2</sub> (110) Surface May Not Form an Efficient Photovoltaic Heterojunction: First-Principles Investigation of Electronic Structures. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2223-2229.	4.6	36
79	Nonradiative Relaxation of Photoexcited Black Phosphorus Is Reduced by Stacking with MoS <sub>2</sub> : A Time Domain ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1830-1835.	4.6	36
80	Strain Controls Charge Carrier Lifetimes in Monolayer WSe <sub>2</sub> : Ab Initio Time Domain Analysis. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7732-7739.	4.6	36
81	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.	12.8	36
82	Atomic geometry and electronic structure of defects in Zn <sub>3</sub> N <sub>2</sub> . <i>Thin Solid Films</i> , 2008, 516, 1297-1301.	1.8	34
83	Hybrid density functional theory description of N- and C-doping of NiO. <i>Journal of Chemical Physics</i> , 2011, 134, 224703.	3.0	34
84	Bidentate Lewis bases are preferred for passivation of MAPbI <sub>3</sub> surfaces: A time-domain ab initio analysis. <i>Nano Energy</i> , 2021, 79, 105491.	16.0	33
85	Controlling Charge Carrier Trapping and Recombination in BiVO <sub>4</sub> with the Oxygen Vacancy Oxidation State. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3514-3521.	4.6	33
86	Time-Domain Ab Initio Analysis of Excitation Dynamics in a Quantum Dot/Polymer Hybrid: Atomistic Description Rationalizes Experiment. <i>Nano Letters</i> , 2015, 15, 4274-4281.	9.1	32
87	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.	5.1	32
88	Quantum Dynamics of Photogenerated Charge Carriers in Hybrid Perovskites: Dopants, Grain Boundaries, Electric Order, and Other Realistic Aspects. <i>ACS Energy Letters</i> , 2017, 2, 1588-1597.	17.4	31
89	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. <i>Journal of Materials Chemistry A</i> , 2022, 10, 8324-8333.	10.3	30
90	New Insights into the Band–Gap Narrowing of (N, P)-Codoped TiO <sub>2</sub> from Hybrid Density Functional Theory Calculations. <i>ChemPhysChem</i> , 2011, 12, 2604-2608.	2.1	29



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91	Lead Vacancy Can Explain the Suppressed Nonradiative Electron-Hole Recombination in FAPbI <sub>3</sub> Perovskite under Iodine-Rich Conditions: A Time-Domain Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6489-6495.	4.6	29
92	Photocarrier dynamics in monolayer phosphorene and bulk black phosphorus. <i>Nanoscale</i> , 2018, 10, 11307-11313.	5.6	29
93	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.	4.6	29
94	Suppressing Oxygen-Induced Deterioration of Metal Halide Perovskites by Alkaline Earth Metal Doping: A Quantum Dynamics Study. <i>Journal of the American Chemical Society</i> , 2022, 144, 5543-5551.	13.7	29
95	First-principles calculation of electronic structure of V-doped anatase TiO <sub>2</sub> . <i>ChemPhysChem</i> , 2010, 11, 2606-2611.	2.1	28
96	Efficient passivation of DY center in CH <sub>3</sub> NH <sub>3</sub> PbBr <sub>3</sub> by chlorine: Quantum molecular dynamics. <i>Nano Research</i> , 2022, 15, 2112-2122.	10.4	28
97	Structural, Electronic, and Optical Properties of Oxygen Defects in Zn <sub>3</sub> N <sub>2</sub> . <i>Journal of Physical Chemistry B</i> , 2007, 111, 3379-3383.	2.6	27
98	Electronic structures of N- and C-doped NiO from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010, 374, 1184-1187.	2.1	27
99	Grain Boundary Facilitates Photocatalytic Reaction in Rutile TiO <sub>2</sub> Despite Fast Charge Recombination: A Time-Domain Ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5884-5889.	4.6	27
100	Weak Distance Dependence of Hot-Electron-Transfer Rates at the Interface between Monolayer MoS <sub>2</sub> and Gold. <i>ACS Nano</i> , 2021, 15, 819-828.	14.6	27
101	Band gap engineering of (N, Si)-codoped TiO <sub>2</sub> from hybrid density functional theory calculations. <i>New Journal of Physics</i> , 2012, 14, 053007.	2.9	26
102	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.	3.0	26
103	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 Ab Initio Study. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1234-1241.	4.6	25
104	Dopant Control of Electron-Hole Recombination in Cesium-Titanium Halide Double Perovskite by Time Domain Ab Initio Simulation: Codoping Supersedes Monodoping. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6907-6914.	4.6	24
105	Unravelling the Effects of A-Site Cations on Nonradiative Electron-Hole Recombination in Lead Bromide Perovskites: Time-Domain ab Initio Analysis. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4834-4840.	4.6	24
106	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.	4.6	24
107	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.	13.8	24
108	Stretchable MoS <sub>2</sub> Artificial Photoreceptors for E-Skin. <i>Advanced Functional Materials</i> , 2022, 32, 2107524.	14.9	24

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109	Electronic properties of F/Zr co-doped anatase TiO <sub>2</sub> photocatalysts from GGA +U calculations. Chemical Physics Letters, 2010, 498, 338-344.	2.6	23
110	Doping-Induced Amorphization, Vacancy, and Gradient Energy Band in SnS <sub>2</sub> Nanosheet Arrays for Improved Photoelectrochemical Water Splitting. Angewandte Chemie, 2019, 131, 6833-6837.	2.0	23
111	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.	4.6	22
112	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. ACS Applied Materials & Interfaces, 2019, 11, 32069-32075.	8.0	22
113	Surface Pb-Dimer Passivated by Molecule Oxygen Notably Suppresses Charge Recombination in CsPbBr <sub>3</sub> Perovskites: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 5499-5506.	4.6	22
114	Covalent Functionalized Black Phosphorus Greatly Inhibits Nonradiative Charge Recombination: A Time Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2020, 11, 478-484.	4.6	22
115	MAI Termination Favors Efficient Hole Extraction and Slow Charge Recombination at the MAPbI <sub>3</sub> /CuSCN Heterojunction. Journal of Physical Chemistry Letters, 2020, 11, 4481-4489.	4.6	22
116	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO <sub>2</sub> (110) Surface. JACS Au, 2022, 2, 234-245.	7.9	22
117	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
118	Hole Localization Inhibits Charge Recombination in Tin-Lead Mixed Perovskites: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 6604-6612.	4.6	21
119	Time-Domain ab Initio Modeling of Electron-Phonon Relaxation in High-Temperature Cuprate Superconductors. Journal of Physical Chemistry Letters, 2017, 8, 193-198.	4.6	20
120	Ferroelastic domains drive charge separation and suppress electron-hole recombination in all-inorganic halide perovskites: time-domain ab initio analysis. Nanoscale Horizons, 2020, 5, 683-690.	8.0	20
121	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.	6.0	20
122	Charge-Compensated Doping Extends Carrier Lifetimes in SrTiO <sub>3</sub> by Passivating Oxygen Vacancy Defects. Journal of Physical Chemistry Letters, 2021, 12, 12040-12047.	4.6	20
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