Run Long

List of Publications by Year
in descending order

190 papers	8,836 citations	36271 51 h-index	56687 83 g-index
192 all docs	192 docs citations	192 times ranked	8829 citing authors

#	Article	IF	Citations
1	Efficient passivation of DY center in CH3NH3PbBr3 by chlorine: Quantum molecular dynamics. Nano Research, 2022, 15, 2112-2122.	5.8	28
2	Bidirectional Light-Driven Ion Transport through Porphyrin Metalâ€“Organic Framework-Based van der Waals Heterostructures via pH-Induced Band Alignment Inversion. CCS Chemistry, 2022, 4, 3329-3341.	4.6	13
3	Stretchable MoS₂ Artificial Photoreceptors for Eâ€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 CH3NH3PbI3 perovskite: A time-domain study. Journal of Chemical Physics, 2022, 156, 014702.	1.2	2
7	Largeâ€Area Printing of Ferroelectric Surface and Superâ€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 MoS₂/WS₂ bilayer: ab initio quantum dynamics. Journal of Materials Chemistry A, 2022, 10, 8324-8333.	5.2	30
9	Correlated organicâ€“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 MoS2 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 Ruddlesdenâ€“Popper Perovskites: A Time-Domain Ab Initio 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) TiO2 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 CH3NH3PbI3 perovskite. Nano Research, 2022, 15, 4765-4772.	5.8	12
17	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO₂(110) Surface. Jacs Au, 2022, 2, 234-245.	3.6	22
18	Unveiling the Valence State of Interstitial Bromine on Charge Carrier Lifetime in CH₃NH₃PbBr₃ by Quantum Dynamics Simulation. Journal of Physical Chemistry Letters, 2022, 13, 4193-4199.	2.1	2

#	Article	IF	Citations
19	Understanding Competitive Photo-Induced Molecular Oxygen Dissociation and Desorption Dynamics atop a Reduced Rutile TiO₂(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 SnS2 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 MAPbI3 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 MoS₂ and Gold. ACS Nano, 2021, 15, 819-828.	7.3	27
25	Doping-Induced Charge Localization Suppresses Electronâ€“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 MoSe₂/WSe₂ Heterostructure. Nano Letters, 2021, 21, 2165-2173.	4.5	46
27	Preventing Superoxide Generation on Molecule-Protected CH₃NH₃PbI₃ 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 Grapheneâ€“MoS₂ 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€Waalsâ€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/TiO₂ Photocatalyst: Atomistic Origin of High Efficiency and Proposed Enhancement by Spin Selection. Jacs Au, 2021, 1, 550-559.	3.6	58
32	Controlling Charge Carrier Trapping and Recombination in BiVO₄ with the Oxygen Vacancy Oxidation State. Journal of Physical Chemistry Letters, 2021, 12, 3514-3521.	2.1	33
33	Marked Passivation Effect of Naphthaleneâ€1,8â€Dicarboximides in Highâ€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/MoS₂ 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

#	Article	IF	Citations
37	Photoinduced Anomalous Electron Transfer Dynamics at a Lateral MoS₂â€“Graphene Covalent Junction. Journal of Physical Chemistry Letters, 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. Journal of Physical Chemistry Letters, 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. Nature Communications, 2021, 12, 5247.	5.8	36
40	Density Functional Theory Half-Electron Self-Energy Correction for Fast and Accurate Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 10886-10892.	2.1	10
41	Charge-Compensated Doping Extends Carrier Lifetimes in SrTiO₃ by Passivating Oxygen Vacancy Defects. Journal of Physical Chemistry Letters, 2021, 12, 12040-12047.	2.1	20
42	Ferroelastic domains drive charge separation and suppress electronâ€“hole recombination in all-inorganic halide perovskites: time-domain ab initio analysis. Nanoscale Horizons, 2020, 5, 683-690.	4.1	20
43	Covalent Functionalized Black Phosphorus Greatly Inhibits Nonradiative Charge Recombination: A Time Domain Ab Initio Study. Journal of Physical Chemistry Letters, 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. Angewandte Chemie - International Edition, 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. Angewandte Chemie, 2020, 132, 4714-4720.	1.6	18
46	Weak temperature-dependent hole injection and electronâ€“hole recombination at the CH₃NH₃PbI₃/NiO heterojunction: a time-domain ab initio study. Journal of Materials Chemistry A, 2020, 8, 607-615.	5.2	16
47	Design of a Z-scheme g-C3N4/CQDs/CdIn2S4 composite for efficient visible-light-driven photocatalytic degradation of ibuprofen. Environmental Pollution, 2020, 259, 113770.	3.7	50
48	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.	2.1	39
49	Isotopic Exchange Extends Charge Carrier Lifetime in Metal Lead Perovskites by Quantum Dynamics Simulations. Journal of Physical Chemistry Letters, 2020, 11, 10298-10305.	2.1	11
50	Unraveling the quantum dynamics origin of high photocatalytic activity in nitrogen-doped anatase TiO₂: time-domain ab initio analysis. Journal of Materials Chemistry A, 2020, 8, 25235-25244.	5.2	19
51	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. ACS Energy Letters, 2020, 5, 3813-3820.	8.8	47
52	Quantum dynamics origin of high photocatalytic activity of mixed-phase anatase/rutile TiO2. Journal of Chemical Physics, 2020, 153, 044706.	1.2	26
53	Photoinduced Dynamics of Charge Carriers in Metal Halide Perovskites from an Atomistic Perspective. Journal of Physical Chemistry Letters, 2020, 11, 7066-7082.	2.1	41
54	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.	6.6	64

#	Article	IF	Citations
55	Influence of tungsten doping on nonradiative electronâ€“hole recombination in monolayer MoSe2 with Se vacancies. Journal of Chemical Physics, 2020, 153, 154701.	1.2	8
56	Oxidation Notably Accelerates Nonradiative Electronâ€“Hole Recombination in MoS2 by Different Mechanisms: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2020, 11, 4086-4092.	2.1	17
57	MAI Termination Favors Efficient Hole Extraction and Slow Charge Recombination at the MAPbI₃/CuSCN Heterojunction. Journal of Physical Chemistry Letters, 2020, 11, 4481-4489.	2.1	22
58	Substrate-free flexible thin film solar cells by graphene-mediated peel-off technology. Journal of Materials Science: Materials in Electronics, 2020, 31, 10279-10287.	1.1	1
59	Two-Dimensional Perovskite Capping Layer Simultaneously Improves the Charge Carriersâ€™ Lifetime and Stability of MAPbI₃ Perovskite: A Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2020, 11, 5100-5107.	2.1	9
60	Covalently Connected Nb₄N_{5â€“x}O_xâ€“MoS₂ Heterocatalysts with Desired Electron Density to Boost Hydrogen Evolution. ACS Nano, 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. Journal of Physical Chemistry Letters, 2020, 11, 1601-1608.	2.1	19
62	Pb dimerization greatly accelerates charge losses in MAPbI3: Time-domain ab initio analysis. Journal of Chemical Physics, 2020, 152, 064707.	1.2	12
63	Direct Growth of Continuous and Uniform MoS₂ Film on SiO₂/Si Substrate Catalyzed by Sodium Sulfate. Journal of Physical Chemistry Letters, 2020, 11, 1570-1577.	2.1	15
64	Reduced-dimensional perovskite photovoltaics with homogeneous energy landscape. Nature Communications, 2020, 11, 1672.	5.8	191
65	The Interplay Between Lead Vacancy and Water Rationalizes the Puzzle of Charge Carrier Lifetimes in CH₃NH₃PbI₃: Timeâ€Domain Ab Initio Analysis. Angewandte Chemie - International Edition, 2020, 59, 13347-13353.	7.2	24
66	The Interplay Between Lead Vacancy and Water Rationalizes the Puzzle of Charge Carrier Lifetimes in CH 3 NH 3 PbI 3 : Timeâ€Domain Ab Initio Analysis. Angewandte Chemie, 2020, 132, 13449-13455.	1.6	0
67	Charge localization control of electronâ€“hole recombination in multilayer two-dimensional Dionâ€“Jacobson hybrid perovskites. Journal of Materials Chemistry A, 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. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	2.2	6
69	Charge localization induced by reorientation of FA cations greatly suppresses nonradiative electron-hole recombination in FAPbI₃ perovskites: A time-domain Ab Initio study. Chinese Journal of Chemical Physics, 2020, 33, 642-648.	0.6	1
70	Ni/Fe Codoped In₂S₃ Nanosheet Arrays Boost Photoâ€Electrochemical Performance of Planar Si Photocathodes. Advanced Energy Materials, 2019, 9, 1902135.	10.2	47
71	Anomalous Temperature-Dependent Charge Recombination in CH₃NH₃PbI₃ Perovskite: Key Roles of Charge Localization and Thermal Effect. ACS Applied Materials & Interfaces, 2019, 11, 32069-32075.	4.0	22
72	Unravelling the Effects of Pressure-Induced Suppressed Electronâ€“Hole Recombination in CsPbBr₃ Perovskite: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 4354-4361.	2.1	19

#	Article	IF	Citations
73	Efficient and Stable Inverted Perovskite Solar Cells Incorporating Secondary Amines. Advanced Materials, 2019, 31, e1903559.	11.1	128
74	A Plasmaâ€Triggered Oâ^'S Bond and Pâ^'N Junction Near the Surface of a SnS₂ Nanosheet Array to Enable Efficient Solar Water Oxidation. Angewandte Chemie - International Edition, 2019, 58, 16668-16675.	7.2	42
75	Aâ€site Cation Engineering for Highly Efficient MAPbI₃ Singleâ€Crystal Xâ€ray Detector. Angewandte Chemie - International Edition, 2019, 58, 17834-17842.	7.2	174
76	Hole Localization Inhibits Charge Recombination in Tinâ€"Lead Mixed Perovskites: Timeâ€"Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 6604-6612.	2.1	21
77	Perovskite Solar Cells: Efficient and Stable Inverted Perovskite Solar Cells Incorporating Secondary Amines (Adv. Mater. 46/2019). Advanced Materials, 2019, 31, 1970330.	11.1	1
78	Ferroelectric Polarization Suppresses Nonradiative Electronâ€"Hole Recombination in CH₃NH₃PbI₃ Perovskites: A Time-Domain ab Initio Study. Journal of Physical Chemistry Letters, 2019, 10, 7237-7244.	2.1	17
79	Aâ€site Cation Engineering for Highly Efficient MAPbI₃ Singleâ€Crystal Xâ€ray Detector. Angewandte Chemie, 2019, 131, 17998-18006.	1.6	15
80	A Plasmaâ€Triggered Oâ^'S Bond and Pâ^'N Junction Near the Surface of a SnS 2 Nanosheet Array to Enable Efficient Solar Water Oxidation. Angewandte Chemie, 2019, 131, 16821-16828.	1.6	11
81	An in situ constructed topological rich vacancy-defect nitrogen-doped nanocarbon as a highly-effective metal-free oxygen catalyst for Liâ€"O₂ batteries. Journal of Materials Chemistry A, 2019, 7, 21918-21926.	5.2	18
82	Ultrafast Charge Separation and Recombination across a Molecule/CsPbBr₃ Quantum Dot Interface from First-Principles Nonadiabatic Molecular Dynamics Simulation. Journal of Physical Chemistry C, 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. Journal of the American Chemical Society, 2019, 141, 15557-15566.	6.6	98
84	Surface Pb-Dimer Passivated by Molecule Oxygen Notably Suppresses Charge Recombination in CsPbBr₃ Perovskites: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 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 CH₃NH₃PbI₃ perovskite: a time-domain ab initio study. Chemical Science, 2019, 10, 10079-10088.	3.7	44
86	Mixed Cs and FA Cations Slow Electronâ€"Hole Recombination in FAPbI₃ Perovskites by Time-Domain Ab Initio Study: Lattice Contraction versus Octahedral Tilting. Journal of Physical Chemistry Letters, 2019, 10, 672-678.	2.1	29
87	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.	2.1	66
88	Doping-Induced Rapid Decoherence Suppresses Charge Recombination in Mono/Divalent Cation Mixed Perovskites from Nonadiabatic Molecular Dynamics Simulation. Journal of Physical Chemistry Letters, 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. Journal of Physical Chemistry Letters, 2019, 10, 2445-2452.	2.1	14
90	Dopingâ€Induced Amorphization, Vacancy, and Gradient Energy Band in SnS₂Nanosheet Arrays for Improved Photoelectrochemical Water Splitting. Angewandte Chemie, 2019, 131, 6833-6837.	1.6	23

#	Article	IF	Citations
91	Dopingâ€Induced Amorphization, Vacancy, and Gradient Energy Band in SnS₂Nanosheet Arrays for Improved Photoelectrochemical Water Splitting. Angewandte Chemie - International Edition, 2019, 58, 6761-6765.	7.2	125
92	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.	6.6	102
93	Symmetry Breaking at MAPbI₃ Perovskite Grain Boundaries Suppresses Charge Recombination: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2019, 10, 1617-1623.	2.1	65
94	Chlorine Passivation of Grain Boundary Suppresses Electronâ€“Hole Recombination in CsPbBr₃ Perovskite by Nonadiabatic Molecular Dynamics Simulation. ACS Applied Energy Materials, 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/WS₂ Junction: A Time Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2019, 10, 1234-1241.	2.1	25
96	Strain Controls Charge Carrier Lifetimes in Monolayer WSe₂: Ab Initio Time Domain Analysis. Journal of Physical Chemistry Letters, 2019, 10, 7732-7739.	2.1	36
97	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. Journal of the American Chemical Society, 2019, 141, 20222-20233.	6.6	42
98	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.	2.1	90
99	Significant enhancement of the performance of hydrogen evolution reaction through shape-controlled synthesis of hierarchical dendrite-like platinum. Journal of Materials Chemistry A, 2018, 6, 8068-8077.	5.2	46
100	Plasmon-Mediated Electron Injection from Au Nanorods into MoS2: Traditional versus Photoexcitation Mechanism. CheM, 2018, 4, 1112-1127.	5.8	71
101	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.	2.1	103
102	Nonadiabatic Molecular Dynamics Simulation of Charge Separation and Recombination at a WS₂/QD Heterojunction. Journal of Physical Chemistry C, 2018, 122, 7041-7050.	1.5	16
103	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain Ab Initio Analysis. Nano Letters, 2018, 18, 2459-2466.	4.5	114
104	Dopant Control of Electronâ€“Hole Recombination in Cesiumâ€“Titanium Halide Double Perovskite by Time Domain Ab Initio Simulation: Codoping Supersedes Monodoping. Journal of Physical Chemistry Letters, 2018, 9, 6907-6914.	2.1	24
105	Layer-Coupled States Facilitate Ultrafast Charge Transfer in a Transition Metal Dichalcogenide Trilayer Heterostructure. Journal of Physical Chemistry Letters, 2018, 9, 5970-5978.	2.1	16
106	Grain Boundary Facilitates Photocatalytic Reaction in Rutile TiO₂ Despite Fast Charge Recombination: A Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 5884-5889.	2.1	27
107	Lead Vacancy Can Explain the Suppressed Nonradiative Electronâ€“Hole Recombination in FAPbI₃ Perovskite under Iodine-Rich Conditions: A Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2018, 9, 6489-6495.	2.1	29
108	Photocarrier dynamics in monolayer phosphorene and bulk black phosphorus. Nanoscale, 2018, 10, 11307-11313.	2.8	29

#	Article	IF	Citations
109	Why Chemical Vapor Deposition Grown MoS₂ 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 Electronâ€“Hole Recombination in Cesiumâ€“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 Electronâ€“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 Layeredâ€Doubleâ€Hydroxide Nanosheets to Feâ€Based Heterostructures for Efficient Visibleâ€Light Photocatalytic Hydrogenation of CO. Advanced Materials, 2018, 30, e1803127.	11.1	100
114	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.	8.8	68
115	Unravelling the Effects of A-Site Cations on Nonradiative Electronâ€“Hole Recombination in Lead Bromide Perovskites: Time-Domain ab Initio Analysis. Journal of Physical Chemistry Letters, 2018, 9, 4834-4840.	2.1	24
116	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.	6.6	132
117	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.	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 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.	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
121	Nonadiabatic charge dynamics in novel solar cell materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1305.	6.2	71
122	Time-Domain ab Initio Modeling of Electronâ€“Phonon Relaxation in High-Temperature Cuprate Superconductors. Journal of Physical Chemistry Letters, 2017, 8, 193-198.	2.1	20
123	Defects Slow Down Nonradiative Electronâ€“Hole Recombination in TiS₃ Nanoribbons: A Time-Domain Ab Initio Study. Journal of Physical Chemistry Letters, 2017, 8, 4522-4529.	2.1	16
124	Disparity in Photoexcitation Dynamics between Vertical and Lateral MoS₂/WSe₂ Heterojunctions: Time-Domain Simulation Emphasizes the Importance of Donorâ€“Acceptor Interaction and Band Alignment. Journal of Physical Chemistry Letters, 2017, 8, 5771-5778.	2.1	52
125	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.	6.6	70
126	Charge Separation and Recombination in Two-Dimensional MoS₂/WS₂: Time-Domain ab Initio Modeling. Chemistry of Materials, 2017, 29, 2466-2473.	3.2	127

#	Article	IF	Citations
127	Sulfur Adatom and Vacancy Accelerate Charge Recombination in MoS₂ but by Different Mechanisms: Time-Domain Ab Initio Analysis. Nano Letters, 2017, 17, 7962-7967.	4.5	136
128	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.	6.6	333
129	Nonradiative Relaxation of Photoexcited Black Phosphorus Is Reduced by Stacking with MoS₂: A Time Domain ab Initio Study. Journal of Physical Chemistry Letters, 2016, 7, 1830-1835.	2.1	36
130	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.	2.1	139
131	Quantum Coherence Facilitates Efficient Charge Separation at a MoS₂/MoSe₂ van der Waals Junction. Nano Letters, 2016, 16, 1996-2003.	4.5	225
132	Nonradiative Electronâ€“Hole Recombination Rate Is Greatly Reduced by Defects in Monolayer Black Phosphorus: Ab Initio Time Domain Study. Journal of Physical Chemistry Letters, 2016, 7, 653-659.	2.1	99
133	Time-Domain Ab Initio Modeling of Photoinduced Dynamics at Nanoscale Interfaces. Annual Review of Physical Chemistry, 2015, 66, 549-579.	4.8	121
134	Time-Domain Ab Initio Analysis of Excitation Dynamics in a Quantum Dot/Polymer Hybrid: Atomistic Description Rationalizes Experiment. Nano Letters, 2015, 15, 4274-4281.	4.5	32
135	Time-Domain Ab Initio Simulation of Energy Transfer in Double-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 12088-12094.	1.5	16
136	Dopants Control Electronâ€“Hole Recombination at Perovskiteâ€“TiO₂ Interfaces: Ab Initio Time-Domain Study. ACS Nano, 2015, 9, 11143-11155.	7.3	108
137	Ultrafast Electron and Hole Relaxation Pathways in Few-Layer MoS₂. Journal of Physical Chemistry C, 2015, 119, 20698-20708.	1.5	47
138	Coherence penalty functional: A simple method for adding decoherence in Ehrenfest dynamics. Journal of Chemical Physics, 2014, 140, 194107.	1.2	86
139	Dimensionality of Nanoscale TiO₂ Determines the Mechanism of Photoinduced Electron Injection from a CdSe Nanoparticle. Nano Letters, 2014, 14, 1790-1796.	4.5	38
140	Ultrafast Carrier Thermalization and Cooling Dynamics in Few-Layer MoS₂. ACS Nano, 2014, 8, 10931-10940.	7.3	236
141	Asymmetry in the Electron and Hole Transfer at a Polymerâ€“Carbon Nanotube Heterojunction. Nano Letters, 2014, 14, 3335-3341.	4.5	67
142	Instantaneous Generation of Charge-Separated State on TiO₂ Surface Sensitized with Plasmonic Nanoparticles. Journal of the American Chemical Society, 2014, 136, 4343-4354.	6.6	221
143	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.	2.1	63
144	Charge separation across P3HT/carbon nanotube interface: First-principles calculations of electronic structures. Chemical Physics Letters, 2014, 597, 45-50.	1.2	3

#	Article	IF	Citations
145	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.	6.6	61
146	Understanding the Electronic Structures of Graphene Quantum Dot Physisorption and Chemisorption onto the TiO₂ (110) Surface: A Firstâ€Principles Calculation. ChemPhysChem, 2013, 14, 579-582.	1.0	36
147	Electronic Structure of Semiconducting and Metallic Tubes in TiO₂/Carbon Nanotube Heterojunctions: Density Functional Theory Calculations. Journal of Physical Chemistry Letters, 2013, 4, 1340-1346.	2.1	55
148	Fullerene Interfaced with a TiO₂(110) Surface May Not Form an Efficient Photovoltaic Heterojunction: First-Principles Investigation of Electronic Structures. Journal of Physical Chemistry Letters, 2013, 4, 2223-2229.	2.1	36
149	Selective Excitation of Atomic-Scale Dynamics by Coherent Exciton Motion in the Non-Bornâ€“Oppenheimer Regime. Journal of Physical Chemistry Letters, 2013, 4, 4260-4266.	2.1	8
150	Band gap engineering of (N, Si)-codoped TiO₂from hybrid density functional theory calculations. New Journal of Physics, 2012, 14, 053007.	1.2	26
151	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.	6.6	226
152	Band gap engineering of double-cation-impurity-doped anatase-titania for visible-light photocatalysts: a hybrid density functional theory approach. Physical Chemistry Chemical Physics, 2011, 13, 13698.	1.3	39
153	Electronic structure of cation-codoped TiO2 for visible-light photocatalyst applications from hybrid density functional theory calculations. Applied Physics Letters, 2011, 98, 142103.	1.5	38
154	Hybrid density functional theory description of N- and C-doping of NiO. Journal of Chemical Physics, 2011, 134, 224703.	1.2	34
155	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.	6.6	120
156	Tailoring the electronic structure of TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>by cation codoping from hybrid density functional theory calculations. Physical Review B, 2011, 83, .	1.1	52
157	Electronic properties of anatase-TiO2 codoped by cation-pairs from hybrid density functional theory calculations. Chemical Physics Letters, 2011, 513, 218-223.	1.2	19
158	New Insights into the Bandâ€Gap Narrowing of (N, P)â€Codoped TiO₂ from Hybrid Density Functional Theory Calculations. ChemPhysChem, 2011, 12, 2604-2608.	1.0	29
159	Synergistic effects on band gap-narrowing in titania by doping from first-principles calculations: density functional theory studies. Materials Research Society Symposia Proceedings, 2011, 1352, 9.	0.1	1
160	Electronic properties of F/Zr co-doped anatase TiO2 photocatalysts from GGA +U calculations. Chemical Physics Letters, 2010, 498, 338-344.	1.2	23
161	Firstâ€principles calculation of electronic structure of Vâ€doped anatase TiO₂. ChemPhysChem, 2010, 11, 2606-2611.	1.0	28
162	Electronic structures of N- and C-doped NiO from first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 1184-1187.	0.9	27

#	Article	IF	Citations
163	First-Principles Calculation of Synergistic (N, P)-Codoping Effects on the Visible-Light Photocatalytic Activity of Anatase TiO₂. Journal of Physical Chemistry C, 2010, 114, 11984-11990.	1.5	55
164	Synergistic Effects on Band Gap-Narrowing in Titania by Codoping from First-Principles Calculations. Chemistry of Materials, 2010, 22, 1616-1623.	3.2	134
165	Electronic Structure and Origin of Visible-Light Activity of C-Doped Cubic In₂O₃ from First-Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 13942-13946.	1.5	8
166	Density functional theory studies of doping in titania. Molecular Simulation, 2010, 36, 618-632.	0.9	12
167	Density functional theory description of the mechanism of ferromagnetism in nitrogen-doped SnO2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 374, 319-322.	0.9	36
168	Band gap engineering of (N,Ta)-codoped TiO2: A first-principles calculation. Chemical Physics Letters, 2009, 478, 175-179.	1.2	95
169	Energetic and Electronic Properties of P Doping at the Rutile TiO₂ (110) Surface from First Principles. Journal of Physical Chemistry C, 2009, 113, 9423-9430.	1.5	18
170	Geometric and Electronic Properties of Sn-Doped TiO₂ from First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 650-653.	1.5	62
171	Structural and electronic properties of iodine-doped anatase and rutile TiO2. Computational Materials Science, 2009, 45, 223-228.	1.4	46
172	Magnetic properties of first-row element-doped ZnS semiconductors: A density functional theory investigation. Physical Review B, 2009, 80, .	1.1	79
173	First-principles calculation of nitrogen-tungsten codoping effects on the band structure of anatase-titania. Applied Physics Letters, 2009, 94, .	1.5	113
174	Synergistic Effects of Bi/S Codoping on Visible Light-Activated Anatase TiO₂ Photocatalysts from First Principles. Journal of Physical Chemistry C, 2009, 113, 8373-8377.	1.5	49
175	First-Principles Study of S Doping at the Rutile TiO₂ (110) Surface. Journal of Physical Chemistry C, 2009, 113, 17464-17470.	1.5	19
176	Energetic and electronic properties of X- (Si, Ge, Sn, Pb) doped TiO2 from first-principles. Physical Chemistry Chemical Physics, 2009, 11, 8165.	1.3	78
177	Characterization of diamond (100) surface with oxygen termination. Applied Surface Science, 2008, 254, 2851-2855.	3.1	13
178	Study of vacancy on diamond (100) (2Ã—1) surface from first-principles. Applied Surface Science, 2008, 254, 6478-6482.	3.1	13
179	Atomic geometry and electronic structure of defects in Zn3N2. Thin Solid Films, 2008, 516, 1297-1301.	0.8	34
180	Structural, Electronic, and Optical Properties of N-doped SnO₂. Journal of Physical Chemistry C, 2008, 112, 9861-9864.	1.5	53

#	Article	IF	Citations
181	First-principles study of heavily B-doped silicon. Computational Materials Science, 2008, 42, 161-167.	1.4	8
182	First-principle prediction of half-metallic ferrimagnetism of the Heusler alloys Mn2CoZ (Z=Al, Ga, Si,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.4	75
183	Effect of B-complexes on lattice structure and electronic properties in heavily boron-doped diamond. Diamond and Related Materials, 2008, 17, 234-239.	1.8	18
184	Structural, Elastic, and Electronic Properties of ReB₂: A First-Principles Calculation. Research Letters in Physics, 2008, 2008, 1-5.	0.2	7
185	First principles studies for formation mechanism and properties of ethylene molecule adsorbing on diamond (100) surface. Journal of Chemical Physics, 2008, 128, 114710.	1.2	2
186	Theoretical Study of Differences between Surface and Bulk Electronic States in Cu Clusters. Solid State Phenomena, 2007, 121-123, 1189-1192.	0.3	0
187	Structural, Electronic, and Optical Properties of Oxygen Defects in Zn3N2. Journal of Physical Chemistry B, 2007, 111, 3379-3383.	1.2	27
188	Structural and Electronic Properties of Oxygen-Adsorbed Diamond (100) Surface. Journal of Physical Chemistry C, 2007, 111, 855-859.	1.5	13
189	Effect of boron on the superconducting transition of heavily doped diamond. Diamond and Related Materials, 2007, 16, 353-358.	1.8	11
190	FERMI-ENERGY AND MINIMUM DIAMETER FOR METALLIC SILVER CLUSTER. International Journal of Modern Physics B, 2005, 19, 2404-2408.	1.0	0