Wei-Hai Fang

List of Publications by Year
in descending order

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		57758	85541
259	7,736	44	71
papers	citations	h-index	g-index

262	262	262	7843
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High-performance artificial nitrogen fixation at ambient conditions using a metal-free electrocatalyst. Nature Communications, 2018, 9, 3485.	12.8	615
2	Ti₃C₂T_x(TÂ= F, OH) MXene nanosheets: conductive 2D catalysts for ambient electrohydrogenation of N₂to NH₃. Journal of Materials Chemistry A, 2018, 6, 24031-24035.	10.3	231
3	BODIPYâ€Based Photodynamic Agents for Exclusively Generating Superoxide Radical over Singlet Oxygen. Angewandte Chemie - International Edition, 2021, 60, 19912-19920.	13.8	186
4	Timeâ€Dependent Afterglow Color in a Singleâ€Component Organic Molecular Crystal. Angewandte Chemie - International Edition, 2020, 59, 10032-10036.	13.8	144
5	Moderate Humidity Delays Electronâ€“Hole Recombination in Hybrid Organicâ€“Inorganic Perovskites: Time-Domain Ab Initio Simulations Rationalize Experiments. Journal of Physical Chemistry Letters, 2016, 7, 3215-3222.	4.6	139
6	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
7	Deep Learning for Nonadiabatic Excited-State Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 6702-6708.	4.6	126
8	Rapid Decoherence Suppresses Charge Recombination in Multi-Layer 2D Halide Perovskites: Time-Domain Ab Initio Analysis. Nano Letters, 2018, 18, 2459-2466.	9.1	114
9	Timeâ€Dependent Afterglow Color in a Singleâ€Component Organic Molecular Crystal. Angewandte Chemie, 2020, 132, 10118-10122.	2.0	103
10	State-specific heavy-atom effect on intersystem crossing processes in 2-thiothymine: A potential photodynamic therapy photosensitizer. Journal of Chemical Physics, 2013, 138, 044315.	3.0	102
11	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
12	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.	4.6	99
13	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
14	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
15	Systematic Theoretical Investigation on the Light Emitter of Firefly. Journal of Chemical Theory and Computation, 2011, 7, 798-803.	5.3	81
16	Designing promising molecules for organic solar cells via machine learning assisted virtual screening. Journal of Materials Chemistry A, 2019, 7, 17480-17488.	10.3	80
17	Electrocatalytic N₂-to-NH₃ conversion using oxygen-doped graphene: experimental and theoretical studies. Chemical Communications, 2019, 55, 7502-7505.	4.1	78
18	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

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19	Ab Initio Determination of Dark Structures in Radiationless Transitions for Aromatic Carbonyl Compounds. Accounts of Chemical Research, 2008, 41, 452-457.	15.6	74
20	Nonadiabatic charge dynamics in novel solar cell materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1305.	14.6	71
21	Plasmon-Mediated Electron Injection from Au Nanorods into MoS2: Traditional versus Photoexcitation Mechanism. CheM, 2018, 4, 1112-1127.	11.7	71
22	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
23	Photodissociation of formic acid. Journal of Chemical Physics, 2000, 113, 1891-1897.	3.0	68
24	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
25	Technical aspects of quantum chemical modeling of enzymatic reactions: the case of phosphotriesterase. Theoretical Chemistry Accounts, 2008, 120, 515-522.	1.4	67
26	Photoisomerization of Arylazopyrazole Photoswitches: Stereospecific Excitedâ€State Relaxation. Angewandte Chemie - International Edition, 2016, 55, 14009-14013.	13.8	65
27	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
28	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
29	ONâ€“OFF Mechanism of a Fluorescent Sensor for the Detection of Zn(II), Cd(II), and Cu(II)Transition Metal Ions. Analytical Chemistry, 2014, 86, 891-899.	6.5	59
30	Tuning excited-state-intramolecular-proton-transfer (ESIPT) process and emission by cocrystal formation: a combined experimental and theoretical study. Chemical Science, 2017, 8, 2086-2090.	7.4	59
31	Dynamics of Oxygen-Independent Photocleavage of Blebbistatin as a One-Photon Blue or Two-Photon Near-Infrared Light-Gated Hydroxyl Radical Photocage. Journal of the American Chemical Society, 2018, 140, 15957-15968.	13.7	58
32	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
33	A Density Functional Theory Investigation of the Simmonsâ"Smith Cyclopropanation Reaction:Â Examination of the Insertion Reaction of Zinc into the Câ"I Bond of CH2I2and Subsequent Cyclopropanation Reactions. Journal of Organic Chemistry, 2002, 67, 154-160.	3.2	56
34	Probing Photocatalytic Nitrogen Reduction to Ammonia with Water on the Rutile TiO₂ (110) Surface by First-Principles Calculations. ACS Catalysis, 2019, 9, 9178-9187.	11.2	56
35	Neutralâ€Eosinâ€Yâ€Photocatalyzed Silane Chlorination Using Dichloromethane. Angewandte Chemie - International Edition, 2019, 58, 12580-12584.	13.8	55
36	Theoretical characterization of the excited-state structures and properties of phenol and its one-water complex. Journal of Chemical Physics, 2000, 112, 1204-1211.	3.0	54

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37	Theoretical Studies of Proton-Transfer Reactions of 2-Hydroxypyridineâ^'(H2O)n (n = 0â^'2) in the Ground and Excited States. Journal of Physical Chemistry A, 2005, 109, 3983-3990.	2.5	53
38	The Origin of the Photoluminescence Enhancement of Goldâ€Doped Silver Nanoclusters: The Importance of Relativistic Effects and Heteronuclear Goldâ€"Silver Bonds. Angewandte Chemie - International Edition, 2018, 57, 9965-9969.	13.8	53
39	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.	4.6	52
40	Elimination of Charge Recombination Centers in Metal Halide Perovskites by Strain. Journal of the American Chemical Society, 2021, 143, 9982-9990.	13.7	52
41	One-Pot Photomediated Giese Reaction/Friedelâ€"Crafts Hydroxyalkylation/Oxidative Aromatization To Access Naphthalene Derivatives from Toluenes and Enones. ACS Catalysis, 2018, 8, 6224-6229.	11.2	51
42	Mechanism of the Visible-Light-Mediated Copper-Catalyzed Coupling Reaction of Phenols and Alkynes. Journal of the American Chemical Society, 2018, 140, 15099-15113.	13.7	50
43	Near-Infrared-Responsive Photo-Driven Nitrogen Fixation Enabled by Oxygen Vacancies and Sulfur Doping in Black TiO_{2â€"x}S_y Nanoplatelets. ACS Applied Materials & Interfaces, 2021, 13, 4975-4983.	8.0	48
44	Atomic Model for Alkali Metal Passivation of Point Defects at Perovskite Grain Boundaries. ACS Energy Letters, 2020, 5, 3813-3820.	17.4	47
45	The Crucial Role of the S1/T2/T1 Intersection in the Relaxation Dynamics of Aromatic Carbonyl Compounds upon nâ†'Ï€* Excitation. ChemPhysChem, 2002, 3, 889-892.	2.1	46
46	Free-triplet generation with improved efficiency in tetracene oligomers through spatially separated triplet pair states. Nature Chemistry, 2021, 13, 559-567.	13.6	46
47	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
48	Theoretical Studies of the Photochemical Dynamics of Acetylacetone:Â Isomerzation, Dissociation, and Dehydration Reactions. Journal of Physical Chemistry A, 2006, 110, 4434-4441.	2.5	44
49	Ab Initio Trajectory Surface-Hopping Study on Ultrafast Deactivation Process of Thiophene. Journal of Physical Chemistry A, 2011, 115, 11544-11550.	2.5	44
50	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.	7.4	44
51	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
52	Visibleâ€Light Photocatalysis of C(sp³)â€H Fluorination by the Uranyl Ion: Mechanistic Insights. Angewandte Chemie - International Edition, 2018, 57, 11812-11816.	13.8	40
53	Polymyxin B Loosens Lipopolysaccharide Bilayer but Stiffens Phospholipid Bilayer. Biophysical Journal, 2020, 118, 138-150.	0.5	40
54	Formation of a mixed-valence Cu(<scp>i</scp>)/Cu(<scp>ii</scp>) metalâ€"organic framework with the full light spectrum and high selectivity of CO₂ photoreduction into CH₄. Chemical Science, 2020, 11, 10143-10148.	7.4	40

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55	Photoinduced Gold(I)â€“Gold(I) Chemical Bonding in Dicyanoaurate Oligomers. Angewandte Chemie - International Edition, 2013, 52, 10281-10285.	13.8	39
56	Photoinduced Proton Transfer and Isomerization in a Hydrogen-Bonded Aromatic Azo Compound: A CASPT2//CASSCF Study. Journal of Physical Chemistry A, 2014, 118, 4732-4739.	2.5	38
57	Theoretical Insight into the Relationship between the Structures of Antimicrobial Peptides and Their Actions on Bacterial Membranes. Journal of Physical Chemistry B, 2015, 119, 850-860.	2.6	38
58	Charge localization control of electronâ€“hole recombination in multilayer two-dimensional Dionâ€“Jacobson hybrid perovskites. Journal of Materials Chemistry A, 2020, 8, 9168-9176.	10.3	38
59	Discrete Stacking of Aromatic Oligoamide Macrocycles. Journal of the American Chemical Society, 2015, 137, 5879-5882.	13.7	37
60	How Photoisomerization Drives Peptide Folding and Unfolding: Insights from QM/MM and MM Dynamics Simulations. Angewandte Chemie - International Edition, 2016, 55, 2067-2072.	13.8	37
61	Mechanistic Insight into the Rhodium-Catalyzed Oâ€“H Insertion Reaction: A DFT Study. Organometallics, 2014, 33, 2448-2456.	2.3	36
62	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.	4.6	36
63	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
64	Concerted Asynchronous Hulaâ€Twist Photoisomerization in the S65T/H148D Mutant of Green Fluorescent Protein. Angewandte Chemie - International Edition, 2014, 53, 8649-8653.	13.8	35
65	Regulatory Mechanism of the Enantioselective Intramolecular Enone [2+2] Photocycloaddition Reaction Mediated by a Chiral Lewis Acid Catalyst Containing Heavy Atoms. Angewandte Chemie - International Edition, 2015, 54, 14295-14298.	13.8	35
66	Photochemistry of Butyrophenone:Â Combined Complete-Active-Space Self-Consistent Field and Density Functional Theory Study of Norrish Type I and II Reactions. Journal of Physical Chemistry A, 2004, 108, 5386-5392.	2.5	34
67	Self-Assembled Carcerand-like Cage with a Thermoregulated Selective Binding Preference for Purification of High-Purity C₆₀ and C₇₀. Journal of Organic Chemistry, 2018, 83, 14667-14675.	3.2	34
68	Theoretical Studies on Excited-State Properties of Au(III) Emitters with Thermally Activated Delayed Fluorescence. Journal of Physical Chemistry C, 2018, 122, 27608-27619.	3.1	33
69	Bidentate Lewis bases are preferred for passivation of MAPbI3 surfaces: A time-domain ab initio analysis. Nano Energy, 2021, 79, 105491.	16.0	33
70	Room-Temperature Phosphorescence and Thermally Activated Delayed Fluorescence in the Pd Complex: Mechanism and Dual Upconversion Channels. Journal of Physical Chemistry Letters, 2021, 12, 5944-5950.	4.6	33
71	Insights into Photodissociation Dynamics of Benzamide and Formanilide from ab Initio Calculations. Journal of the American Chemical Society, 2004, 126, 8976-8980.	13.7	32
72	Integrating Machine Learning with the Multilayer Energy-Based Fragment Method for Excited States of Large Systems. Journal of Physical Chemistry Letters, 2019, 10, 7836-7841.	4.6	32

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73	Regulatory Mechanism and Kinetic Assessment of Energy Transfer Catalysis Mediated by Visible Light. ACS Catalysis, 2019, 9, 3672-3684.	11.2	31
74	Excitonâ€“Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 3721-3729.	5.3	31
75	QM and ONIOM studies on thermally activated delayed fluorescence of copper(<scp>i</scp>) complexes in gas phase, solution, and crystal. Physical Chemistry Chemical Physics, 2018, 20, 24955-24967.	2.8	30
76	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
77	Nonadiabatic molecular dynamics simulation: An approach based on quantum measurement picture. AIP Advances, 2014, 4, .	1.3	29
78	Nanodomain Formation of Ganglioside GM1 in Lipid Membrane: Effects of Cholera Toxin-Mediated Cross-Linking. Langmuir, 2015, 31, 9105-9114.	3.5	29
79	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
80	Quantum Mechanics/Molecular Mechanics Study on the Photoreactions of Darkâ€•and Lightâ€Adapted States of a Blueâ€Light YtvA LOV Photoreceptor. Angewandte Chemie - International Edition, 2017, 56, 9341-9345.	13.8	28
81	Theoretical Insights into Interfacial Electron Transfer between Zinc Phthalocyanine and Molybdenum Disulfide. Journal of Physical Chemistry A, 2018, 122, 9587-9596.	2.5	28
82	Efficient passivation of DY center in CH3NH3PbBr3 by chlorine: Quantum molecular dynamics. Nano Research, 2022, 15, 2112-2122.	10.4	28
83	Short-time dynamics of 2-thiouracil in the light absorbing S2(Ï€Ï€â^—) state. Journal of Chemical Physics, 2015, 143, 175103.	3.0	27
84	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.	4.6	27
85	Identifying and Modulating Accidental Fermi Resonance: 2D IR and DFT Study of 4-Azido-<scp>l</scp>-phenylalanine. Journal of Physical Chemistry B, 2018, 122, 8122-8133.	2.6	27
86	Efficient Construction of Excited-State Hessian Matrices with Machine Learning Accelerated Multilayer Energy-Based Fragment Method. Journal of Physical Chemistry A, 2020, 124, 5684-5695.	2.5	27
87	Effects of induced tension and electrostatic interactions on the mechanisms of antimicrobial peptide translocation across lipid bilayer. Soft Matter, 2009, 5, 3312.	2.7	26
88	Insights into the mechanistic photodissociation of methyl formate. Journal of Chemical Physics, 2010, 132, 034306.	3.0	26
89	Reformulating time-dependent density functional theory with non-orthogonal localized molecular orbitals. Physical Chemistry Chemical Physics, 2010, 12, 416-421.	2.8	26
90	Three-state conical intersection optimization methods: development and implementation at QM/MM level. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	26

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91	A multi-layer energy-based fragment method for excited states and nonadiabatic dynamics. Physical Chemistry Chemical Physics, 2019, 21, 22695-22699.	2.8	26
92	Highly Conducting Organicâ€“Inorganic Hybrid Copper Sulfides Cu_xC₆S₆ (x=4 or 5.5): Ligandâ€Based Oxidationâ€Induced Chemical and Electronic Structure Modulation. Angewandte Chemie - International Edition, 2020, 59, 22602-22609.	13.8	26
93	Ab initio implementation of quantum trajectory mean-field approach and dynamical simulation of the N2CO photodissociation. Journal of Chemical Physics, 2015, 143, 194107.	3.0	25
94	Early-Time Excited-State Relaxation Dynamics of Iridium Compounds: Distinct Roles of Electron and Hole Transfer. Journal of Physical Chemistry A, 2018, 122, 5518-5532.	2.5	25
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.	4.6	25
96	Dissipative Particle Dynamics Simulations for Phospholipid Membranes Based on a Four-To-One Coarse-Grained Mapping Scheme. PLoS ONE, 2016, 11, e0154568.	2.5	25
97	Conical Intersection Is Responsible for the Fluorescence Disappearance below 365 nm in Cyclopropanone. Journal of Physical Chemistry A, 2010, 114, 730-734.	2.5	24
98	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.	4.6	24
99	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.	4.6	24
100	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.	13.8	24
101	Ab Initio Based Surface-Hopping Dynamics Study on Ultrafast Internal Conversion in Cyclopropanone. Journal of Physical Chemistry A, 2011, 115, 1547-1555.	2.5	23
102	Energy Resonance Crossing Controls the Photoluminescence of Europium Antenna Probes. Angewandte Chemie - International Edition, 2017, 56, 7986-7990.	13.8	23
103	Photocatalytic Reduction of Carbon Dioxide to Methane at the Pd-Supported TiO₂ Interface: Mechanistic Insights from Theoretical Studies. ACS Catalysis, 2022, 12, 8558-8571.	11.2	23
104	Theoretical Characterization of the Structures and Reactivity of 7-Hydroxyquinolineâˆ™(H2O)n(n= 1â€“3) Complexes. Journal of Physical Chemistry A, 1999, 103, 5567-5573.	2.5	22
105	Ab initio studies of dissociation pathways on the ground- and excited-state potential energy surfaces for HFCO. Journal of Chemical Physics, 2001, 115, 5411-5417.	3.0	22
106	Combined CASSCF and MR-CI Study on Photoinduced Dissociation and Isomerization of Acryloyl Chloride. Journal of Physical Chemistry A, 2006, 110, 11839-11846.	2.5	22
107	pH- and Wavelength-Dependent Photodecarboxylation of Ketoprofen. Organic Letters, 2011, 13, 5472-5475.	4.6	22
108	Photoinduced Carrier Dynamics at the Interface of Pentacene and Molybdenum Disulfide. Journal of Physical Chemistry A, 2019, 123, 7693-7703.	2.5	22

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109	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.	4.6	22
110	Nonadiabatic Dynamics Simulations Reveal Distinct Effects of the Thickness of PTB7 on Interfacial Electron and Hole Transfer Dynamics in PTB7@MoS₂ Heterostructures. Journal of Physical Chemistry Letters, 2019, 10, 2949-2956.	4.6	22
111	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
112	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
113	CO Adsorbate Promotes Polaron Photoactivity on the Reduced Rutile TiO₂(110) Surface. Jacs Au, 2022, 2, 234-245.	7.9	22
114	Computational Insight into Metallated Graphynes as Single Atom Electrocatalysts for Nitrogen Fixation. ACS Applied Materials & Interfaces, 2022, 14, 27861-27872.	8.0	22
115	Energy Transfer Tunes Phosphorescent Color of Singleâ€Dopant White OLEDs. Chemistry - A European Journal, 2011, 17, 13971-13977.	3.3	21
116	How the Antimicrobial Peptides Kill Bacteria: Computational Physics Insights. Communications in Computational Physics, 2012, 11, 709-725.	1.7	21
117	Mechanism of Inhibition of Human Islet Amyloid Polypeptide-Induced Membrane Damage by a Small Organic Fluorogen. Scientific Reports, 2016, 6, 21614.	3.3	21
118	Spinâ€“Orbit Coupling Accelerates the Photoinduced Interfacial Electron Transfer in a Fullerene-Based Perovskite Heterojunction. Journal of Physical Chemistry Letters, 2021, 12, 1131-1137.	4.6	21
119	Density Functional Theory Investigation of the Reactivity of LiCH2I and Iodomethylzinc Phenoxide Cyclopropanation Reagents with Olefins. Organometallics, 2002, 21, 5901-5910.	2.3	20
120	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.	8.0	20
121	Quantum computation of molecular response properties. Physical Review Research, 2020, 2, .	3.6	20
122	Theoretical characterization of the ground- and excited-state structures and properties of indole-(H2O)n (n=1,2) complexes. Journal of Chemical Physics, 1999, 111, 5361-5367.	3.0	19
123	Phosphorescent mechanism for single-dopant white OLED of FPt: electronic structure and electron exchange-induced energy transfer. Journal of Materials Chemistry C, 2013, 1, 4227.	5.5	19
124	Mechanism of the Enantioselective Intramolecular [2 + 2] Photocycloaddition Reaction of Coumarin Catalyzed by a Chiral Lewis Acid: Comparison with Enone Substrates. Journal of Organic Chemistry, 2016, 81, 7093-7101.	3.2	19
125	Photoinduced relaxation dynamics of nitrogen-capped silicon nanoclusters: a TD-DFT study. Molecular Physics, 2018, 116, 869-884.	1.7	19
126	MS-CASPT2 Studies on the Photophysics of Selenium-Substituted Guanine Nucleobase. ACS Omega, 2019, 4, 9769-9777.	3.5	19

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127	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.	10.3	19
128	High-Lying 3¹A_g Dark-State-Mediated Singlet Fission. Journal of the American Chemical Society, 2021, 143, 5691-5697.	13.7	19
129	How Photoisomerization Drives Peptide Folding and Unfolding: Insights from QM/MM and MM Dynamics Simulations. Angewandte Chemie, 2016, 128, 2107-2112.	2.0	18
130	Peptide-Lipid Interaction Sites Affect Vesiclesâ€™ Responses to Antimicrobial Peptides. Biophysical Journal, 2018, 115, 1518-1529.	0.5	18
131	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
132	Nonadiabatic Exciton and Charge Separation Dynamics at Interfaces of Zinc Phthalocyanine and Fullerene: Orientation Does Matter. Journal of Physical Chemistry A, 2020, 124, 7388-7398.	2.5	18
133	Correlated organicâ€“inorganic motion enhances stability and charge carrier lifetime in mixed halide perovskites. Nanoscale, 2022, 14, 4644-4653.	5.6	18
134	Effects of Antimicrobial Peptide Revealed by Simulations: Translocation, Pore Formation, Membrane Corrugation and Euler Buckling. International Journal of Molecular Sciences, 2013, 14, 7932-7958.	4.1	17
135	The Position of the N Atom Plays a Significant Role for Excited-State Decay of Heterocycles. Journal of Physical Chemistry Letters, 2017, 8, 1019-1024.	4.6	17
136	Nonadiabatic Curve-Crossing Model for the Visible-Light Photoredox Catalytic Generation of Radical Intermediate via a Concerted Mechanism. ACS Catalysis, 2018, 8, 7388-7396.	11.2	17
137	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.	4.6	17
138	Hydrogen-Bonding Interaction Regulates Photoisomerization of a Single-Bond-Rotation Locked Photoactive Yellow Protein Chromophore in Protein. Journal of Physical Chemistry Letters, 2020, 11, 2470-2476.	4.6	17
139	Selectivity of the Î± and Î² bond fissions for bromoacetyl chloride upon nâ†'Ï€* excitation: A combined complete-active-space self-consistent field and multireference configuration interaction study. Journal of Chemical Physics, 2002, 117, 8745-8753.	3.0	16
140	Importance of the Intramolecular Hydrogen Bond on the Photochemistry of Anionic Hydroquinone (FADH^{â¾}) in DNA Photolyase. Journal of Physical Chemistry Letters, 2010, 1, 743-747.	4.6	16
141	Mechanistic Photodissociation of Glycolaldehyde: Insights from Ab Initio and RRKM Calculations. ChemPhysChem, 2011, 12, 1351-1357.	2.1	16
142	A comprehensive study of isomerization and protonation reactions in the photocycle of the photoactive yellow protein. Physical Chemistry Chemical Physics, 2014, 16, 25263-25272.	2.8	16
143	Multiple-State Nonadiabatic Dynamics Simulation of Photoisomerization of Acetylacetone with the Direct ab Initio QTMF Approach. Journal of Chemical Theory and Computation, 2017, 13, 2717-2729.	5.3	16
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