Wei Li

List of Publications by Year in descending order

39 papers	1,468 citations	304743 22 h-index	315739 38 g-index
39 all docs	39 docs citations	39 times ranked	1548 citing authors

#	Article	IF	Citations
1	Hole Trapping by Iodine Interstitial Defects Decreases Free Carrier Losses in Perovskite Solar Cells: A Time-Domain Ab Initio Study. ACS Energy Letters, 2017, 2, 1270-1278.	17.4	151
2	Control of Charge Recombination in Perovskites by Oxidation State of Halide Vacancy. Journal of the American Chemical Society, 2018, 140, 15753-15763.	13.7	129
3	Spinâ€“Orbit Interactions Greatly Accelerate Nonradiative Dynamics in Lead Halide Perovskites. ACS Energy Letters, 2018, 3, 2159-2166.	17.4	114
4	Elastic properties and thermal expansion of lead-free halide double perovskite Cs2AgBiBr6. Computational Materials Science, 2018, 141, 49-58.	3.0	87
5	Ab initio nonadiabatic molecular dynamics of charge carriers in metal halide perovskites. Nanoscale, 2021, 13, 10239-10265.	5.6	70
6	Time-Domain ab Initio Analysis Rationalizes the Unusual Temperature Dependence of Charge Carrier Relaxation in Lead Halide Perovskite. ACS Energy Letters, 2018, 3, 2713-2720.	17.4	68
7	Anharmonicity Extends Carrier Lifetimes in Lead Halide Perovskites at Elevated Temperatures. Journal of Physical Chemistry Letters, 2019, 10, 6219-6226.	4.6	66
8	Influence of Defects on Excited-State Dynamics in Lead Halide Perovskites: Time-Domain ab Initio Studies. Journal of Physical Chemistry Letters, 2019, 10, 3788-3804.	4.6	66
9	What Makes Hydroxamate a Promising Anchoring Group in Dye-Sensitized Solar Cells? Insights from Theoretical Investigation. Journal of Physical Chemistry Letters, 2014, 5, 3992-3999.	4.6	61
10	Passivating Detrimental DX Centers in CH₃NH₃PbI₃ for Reducing Nonradiative Recombination and Elongating Carrier Lifetime. Advanced Materials, 2020, 32, e1906115.	21.0	53
11	Theoretical investigation of triphenylamine-based sensitizers with different Ï€-spacers for DSSC. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 1144-1151.	3.9	46
12	Electronic structures and elastic properties of a family of metal-free perovskites. Materials Chemistry Frontiers, 2019, 3, 1678-1685.	5.9	46
13	Planar amine-based dye features the rigidified O-bridged dithiophene Ï€-spacer: A potential high-efficiency sensitizer for dye-sensitized solar cells application. Journal of Power Sources, 2015, 275, 207-216.	7.8	45
14	Theoretical investigation and design of high-efficiency dithiafulvenyl-based sensitizers for dye-sensitized solar cells: the impacts of elongating Ï€-spacers and rigidifying dithiophene. Physical Chemistry Chemical Physics, 2014, 16, 9458.	2.8	40
15	Anti-correlation between Band gap and Carrier Lifetime in Lead Halide Perovskites under Compression Rationalized by Ab Initio Quantum Dynamics. Chemistry of Materials, 2020, 32, 4707-4715.	6.7	36
16	Anionic ancillary ligands in cyclometalated Ru(<scp>ii</scp>) complex sensitizers improve photovoltaic efficiency of dye-sensitized solar cells: insights from theoretical investigations. Journal of Materials Chemistry A, 2017, 5, 15567-15577.	10.3	33
17	Promising pyridinium ylide based anchors towards high-efficiency dyes for dye-sensitized solar cells applications: Insights from theoretical investigations. Electrochimica Acta, 2018, 283, 1798-1805.	5.2	33
18	Rational design of metal-free organic D-Ï€-A dyes in dye-sensitized solar cells: Insight from density functional theory (DFT) and time-dependent DFT (TD-DFT) investigations. Organic Electronics, 2018, 59, 131-139.	2.6	28

#	Article	IF	Citations
19	Highly-efficient sensitizer with zinc porphyrin as building block: Insights from DFT calculations. Solar Energy, 2018, 173, 283-290.	6.1	27
20	Theoretical investigation of the adsorption, IR, and electron injection of hydroxamate anchor at the TiO₂ anatase (1 0 1) surface. RSC Advances, 2014, 4, 19690-19693.	3.6	26
21	How does graphene enhance the photoelectric conversion efficiency of dye sensitized solar cells? An insight from a theoretical perspective. Journal of Materials Chemistry A, 2019, 7, 2730-2740.	10.3	26
22	Atomistic Mechanism of Passivation of Halide Vacancies in Lead Halide Perovskites by Alkali Ions. Chemistry of Materials, 2021, 33, 1285-1292.	6.7	26
23	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
24	Shock wave propagation, plasticity, and void collapse in open-cell nanoporous Ta. Physical Chemistry Chemical Physics, 2018, 20, 28039-28048.	2.8	19
25	Novel ultra-high-temperature zero-thermal quenching plant-protecting type blue-green dual-emission KAl₁₁O₁₇:Eu²⁺,Mn²⁺ phosphors for urban ecological lighting. Journal of Materials Chemistry C, 2022, 10, 3461-3471.	5.5	19
26	Identifying and Passivating Killer Defects in Pb-Free Double Cs₂AgBiBr₆ Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 10581-10588.	4.6	17
27	Theoretical study on organic dyes with tunable Ï€-spacers for dye-sensitized solar cells: Inspired by the organic polymer photovoltaics. Chemical Physics Letters, 2019, 719, 39-44.	2.6	13
28	Elucidating the Influence of Sulfur Vacancies on Nonradiative Recombination Dynamics in Cu₂ZnSnS₄ Solar Absorbers. Journal of Physical Chemistry Letters, 2020, 11, 10354-10361.	4.6	13
29	Unraveling photoexcitation dynamics at â€œdots-in-a-perovskiteâ€•heterojunctions from first-principles. Journal of Materials Chemistry A, 2019, 7, 18012-18019.	10.3	12
30	Weak Anharmonicity Rationalizes the Temperature-Driven Acceleration of Nonradiative Dynamics in Cu₂ZnSnS₄Photoabsorbers. ACS Applied Materials & Interfaces, 2021, 13, 61365-61373.	8.0	11
31	Regulating ancillary ligands of Ru(<scp>ii</scp>) complexes with square-planar quadridentate ligands for more efficient sensitizers in dye-sensitized solar cells: insights from theoretical investigations. Physical Chemistry Chemical Physics, 2016, 18, 29591-29599.	2.8	9
32	Theoretical design of porphyrin dyes with electron-deficit heterocycles towards near-IR light sensitization in dye-sensitized solar cells. Solar Energy, 2019, 188, 742-749.	6.1	9
33	Intrinsic strain-induced segregation in multiply twinned Cuâ€“Pt icosahedra. Physical Chemistry Chemical Physics, 2019, 21, 4802-4809.	2.8	9
34	Resolving the mechanism of oxygen vacancy mediated nonradiative charge recombination in monoclinic bismuth vanadate. Chemical Physics Letters, 2021, 766, 138342.	2.6	9
35	Influence of an exciton-delocalizing ligand on the structural, electronic, and spectral features of the Cd₃₃S₃₃ quantum dot: insights from computational studies. Journal of Materials Chemistry C, 2018, 6, 8751-8761.	5.5	7
36	Stability, Aromaticity, and Photophysical Behaviors of Macrocyclic Molecules: A Theoretical Analysis. Frontiers in Chemistry, 2020, 8, 776.	3.6	6

#	Article	IF	Citations
37	High-performance Ruddlesdenâ€“Popper two-dimensional perovskite solar cells via solution processed inorganic charge transport layers. Physical Chemistry Chemical Physics, 2022, 24, 15912-15919.	2.8	6
38	Nonadiabatic Molecular Dynamics with Extended Density Functional Tight-Binding: Application to Nanocrystals and Periodic Solids. Journal of Chemical Theory and Computation, 2022, 18, 5157-5180.	5.3	6
39	Effect of chlorine vacancy on the electronic and optical properties of CsSnCl3 perovskites for optoelectronic applications. Chemical Physics Letters, 2022, 794, 139397.	2.6	5