Fan Zheng

List of Publications by Year
in descending order

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Version: 2024-02-01

26 papers	2,511 citations	394286 19 h-index	552653 26 g-index
26 all docs	26 docs citations	26 times ranked	4302 citing authors

#	Article	IF	Citations
1	Local Polar Fluctuations in Lead Halide Perovskite Crystals. Physical Review Letters, 2017, 118, 136001.	2.9	489
2	Rashba Spinâ€“Orbit Coupling Enhanced Carrier Lifetime in CH₃NH₃PbI₃. Nano Letters, 2015, 15, 7794-7800.	4.5	438
3	Ferroelectric Domain Wall Induced Band Gap Reduction and Charge Separation in Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 693-699.	2.1	293
4	Shift current bulk photovoltaic effect in polar materialsâ€”hybrid and oxide perovskites and beyond. Npj Computational Materials, 2016, 2, .	3.5	246
5	First-Principles Calculation of the Bulk Photovoltaic Effect in CH₃NH₃PbI₃ and CH₃NH₃PbI_{3â€“x}Cl_x. Journal of Physical Chemistry Letters, 2015, 6, 31-37.	2.1	177
6	Enhancing ferroelectric photovoltaic effect by polar order engineering. Science Advances, 2018, 4, eaat3438.	4.7	152
7	Large polaron formation and its effect on electron transport in hybrid perovskites. Energy and Environmental Science, 2019, 12, 1219-1230.	15.6	106
8	Investigation and mitigation of degradation mechanisms in Cu2O photoelectrodes for CO2 reduction to ethylene. Nature Energy, 2021, 6, 1124-1132.	19.8	85
9	Photoferroelectric and Photopiezoelectric Properties of Organometal Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 1460-1465.	2.1	73
10	Theoretical Investigation of 2D Conductive Microporous Coordination Polymers as Liâ€“S Battery Cathode with Ultrahigh Energy Density. Advanced Energy Materials, 2018, 8, 1801823.	10.2	63
11	Substantial bulk photovoltaic effect enhancement via nanolayering. Nature Communications, 2016, 7, 10419.	5.8	62
12	Borophosphene: A New Anisotropic Dirac Cone Monolayer with a High Fermi Velocity and a Unique Self-Doping Feature. Journal of Physical Chemistry Letters, 2019, 10, 6656-6663.	2.1	45
13	First-principles calculation of the bulk photovoltaic effect in the polar compounds LiAsS2, LiAsSe2, and NaAsSe2. Journal of Chemical Physics, 2014, 141, 204704.	1.2	44
14	Material Innovation in Advancing Organometal Halide Perovskite Functionality. Journal of Physical Chemistry Letters, 2015, 6, 4862-4872.	2.1	37
15	Phonon Influence on Bulk Photovoltaic Effect in the Ferroelectric Semiconductor GeTe. Physical Review Letters, 2018, 121, 017402.	2.9	30
16	Intermolecular Interactions in Hybrid Perovskites Understood from a Combined Density Functional Theory and Effective Hamiltonian Approach. ACS Energy Letters, 2017, 2, 937-942.	8.8	28
17	Frequency-dependent dielectric function of semiconductors with application to physisorption. Physical Review B, 2017, 95, .	1.1	25
18	Ultrafast Hot Carrier Injection in Au/GaN: The Role of Band Bending and the Interface Band Structure. Journal of Physical Chemistry Letters, 2019, 10, 6174-6183.	2.1	23

#	Article	IF	Citations
19	itio Investigation of Charge Trapping Across the Crystalline- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Si</mml:mi></mml:math> â€“Amorphous- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Interf	1.5	22
20	Screened van der Waals correction to density functional theory for solids. Physical Review Materials, 2017, 1, .	0.9	19
21	Effects of the c-Si/a-SiO₂ interfacial atomic structure on its band alignment: an ab initio study. Physical Chemistry Chemical Physics, 2017, 19, 32617-32625.	1.3	17
22	Giant Bulk Photovoltaic Effect in Vinylene-Linked Hybrid Heterocyclic Polymer. Journal of Physical Chemistry C, 2017, 121, 6500-6507.	1.5	15
23	Solid 3D Liâ€“S Battery Design via Stacking 2D Conductive Microporous Coordination Polymers and Amorphous Liâ€“S Layers. Chemistry of Materials, 2020, 32, 1974-1982.	3.2	11
24	Distribution of alkali cations near the Cu (111) surface in aqueous solution. Journal of Materials Chemistry A, 2020, 8, 24428-24437.	5.2	6
25	Exploring non-adiabaticity to CO reduction reaction through ab initio molecular dynamics simulation. APL Materials, 2020, 8, 041115.	2.2	4
26	Substantial optical dielectric enhancement by volume compression inLiAsSe2. Physical Review B, 2016, 93, .	1.1	1