Zhaohui Zhou

List of Publications by Year
in descending order

52	11,624	249298	206121
papers	citations	26 h-index	51 g-index

53	53	53	15747
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomically Dispersed Janus Nickel Sites on Red Phosphorus for Photocatalytic Overall Water Splitting. Angewandte Chemie - International Edition, 2022, 61, .	7.2	43
2	Photoinduced small electron polarons generation and recombination in hematite. Npj Computational Materials, 2022, 8, .	3.5	10
3	H2S Dissociation on Defective or Strained Fe (110) and Subsequent Formation of Iron Sulfides: A Density Functional Theory Study. Surface Science, 2021, 709, 121835.	0.8	1
4	Strain effect on oxygen evolution reaction of the SrTiO3 (0 0 1) surface. Applied Physics Letters, 2021, 119, .	1.5	4
5	Regulate chemical environment to control the formation of defects on Ta3N5 (1 1 0) surface: From theoretical perspectives. Chemical Physics Letters, 2021, 782, 139026.	1.2	2
6	Quantum dynamics origin of high photocatalytic activity of mixed-phase anatase/rutile TiO2. Journal of Chemical Physics, 2020, 153, 044706.	1.2	26
7	Photoinduced Superhydrophilicity of Anatase TiO₂ Surface Uncovered by First-Principles Molecular Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 7590-7594.	2.1	10
8	Firstâ€Principles Investigation of Î²â€FeOOH for Hydrogen Evolution: Identifying Reactive Sites and Boosting Surface Reactions. Chemistry - A European Journal, 2020, 26, 7118-7123.	1.7	6
9	Improved description of hematite surfaces by the SCAN functional. Journal of Chemical Physics, 2020, 152, 024706.	1.2	13
10	Which phase of iron oxyhydroxides (FeOOH) is more competent in overall water splitting as a photocatalyst, goethite, akaganeite or lepidocrocite? A DFT-based investigation. Computational Materials Science, 2019, 169, 109110.	1.4	28
11	Why Silicon Doping Accelerates Electron Polaron Diffusion in Hematite. Journal of the American Chemical Society, 2019, 141, 20222-20233.	6.6	42
12	First-Principles Study on Stability and HER Activity of Noble Metal Single Atoms on TiO₂: The Effect of Loading Density. Journal of Physical Chemistry C, 2018, 122, 2546-2553.	1.5	27
13	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
14	Control of Charge Recombination in Perovskites by Oxidation State of Halide Vacancy. Journal of the American Chemical Society, 2018, 140, 15753-15763.	6.6	129
15	New Theoretical Strategy for the Correlation of Oxygen Evolution Performance and Metal Catalysts Adsorption at BiVO₄ Surfaces. Journal of Physical Chemistry C, 2018, 122, 25195-25203.	1.5	10
16	Effect of Water Adsorption on the Interfacial Structure and Band Edge Alignment of Anatase TiO₂(001)/Water by First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2018, 122, 26965-26973.	1.5	22
17	Molten Ag₂SO₄â€based Ionâ€Exchange Preparation of Ag_{0.5}La_{0.5}TiO₃ for Photocatalytic O₂ Evolution. Chemistry - an Asian Journal, 2017, 12, 882-889.	1.7	8
18	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

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19	LaTiO2Nâ€“LaCrO3: continuous solid solutions towards enhanced photocatalytic H2 evolution under visible-light irradiation. Dalton Transactions, 2017, 46, 10685-10693.	1.6	6
20	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
21	One-pot preparation of porous Cr2O3/g-C3N4 composites towards enhanced photocatalytic H2 evolution under visible-light irradiation. International Journal of Hydrogen Energy, 2017, 42, 4651-4659.	3.8	45
22	NH3-treated MoS2 nanosheets as photocatalysts for enhanced H2 evolution under visible-light irradiation. Journal of Alloys and Compounds, 2016, 688, 368-375.	2.8	35
23	A comparative study on structural and electronic properties and formation energy of bulk Î±-Fe2O3 using first-principles calculations with different density functionals. Computational Materials Science, 2016, 113, 117-122.	1.4	15
24	Spontaneous photoelectric field-enhancement effect prompts the low cost hierarchical growth of highly ordered heteronanostructures for solar water splitting. Nano Research, 2016, 9, 1561-1569.	5.8	51
25	Co₃(OH)₂(HPO₄)₂ as a novel photocatalyst for O₂ evolution under visible-light irradiation. Catalysis Science and Technology, 2016, 6, 8080-8088.	2.1	27
26	Novel cubic-phase pyrochlore Sb(III)2Sn(IV)2O7 transformed from Sn(II)2Sb(V)2O7: First-principles calculation-based prediction and experimental evidence. Materials and Design, 2016, 110, 207-213.	3.3	5
27	The effect of thermal annealing on the interfacial properties and photoelectrochemical performance of Ti doped Fe₂O₃ nanowire arrays. RSC Advances, 2016, 6, 99851-99858.	1.7	5
28	Exposing the Dynamics and Energetics of the N-Heterocyclic Carbeneâ€“Nanocrystal Interface. Journal of the American Chemical Society, 2016, 138, 14844-14847.	6.6	34
29	Understanding divergent behaviors in the photocatalytic hydrogen evolution reaction on CdS and ZnS: a DFT based study. Physical Chemistry Chemical Physics, 2016, 18, 16862-16869.	1.3	36
30	Solution growth of Ta-doped hematite nanorods for efficient photoelectrochemical water splitting: a tradeoff between electronic structure and nanostructure evolution. Physical Chemistry Chemical Physics, 2016, 18, 3846-3853.	1.3	58
31	Eosin Y-sensitized nanosheet-stacked hollow-sphere TiO2 for efficient photocatalytic H2 production under visible-light irradiation. Journal of Nanoparticle Research, 2015, 17, 1.	0.8	8
32	Revisiting the Zinc-Blende/Wurtzite Heterocrystalline Structure in CdS. Advances in Condensed Matter Physics, 2014, 2014, 1-7.	0.4	5
33	Configuration dependence of the properties of Cd_{1â€“x}<scp>Z</scp>n_x<scp>S</scp> solid solutions by firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2014, 251, 655-660.	0.7	5
34	A Firstâ€Principles Investigation on Microscopic Atom Distribution and Configurationâ€Averaged Properties in Cd_{1â^'x}Zn_xS Solid Solutions. ChemPhysChem, 2014, 15, 3125-3132.	1.0	6
35	Physical and photoelectrochemical properties of Zr-doped hematite nanorod arrays. Nanoscale, 2013, 5, 9867.	2.8	106
36	Twin-induced one-dimensional homojunctions yield high quantum efficiency for solar hydrogen generation. Nature Communications, 2013, 4, 2278.	5.8	325

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37	A novel Sn2Sb2O7 nanophotocatalyst for visible-light-driven H2 evolution. Nano Research, 2012, 5, 576-583.	5.8	22
38	ABO3-based photocatalysts for water splitting. Progress in Natural Science: Materials International, 2012, 22, 592-615.	1.8	243
39	Tin(II) Antimonates with Adjustable Compositions: Effects of Bandâ€Gaps and Nanostructures on Visibleâ€Lightâ€Driven Photocatalytic H₂ Evolution. ChemCatChem, 2012, 4, 1389-1396.	1.8	13
40	Twins in Cd1â^'xZnxS solid solution: Highly efficient photocatalyst for hydrogen generation from water. Energy and Environmental Science, 2011, 4, 1372.	15.6	332
41	First-principles study on absolute band edge positions for IIâ€“VI semiconductors at (110) surface. Chemical Physics Letters, 2011, 513, 72-76.	1.2	9
42	Nanostructured WO₃/BiVO₄Heterojunction Films for Efficient Photoelectrochemical Water Splitting. Nano Letters, 2011, 11, 1928-1933.	4.5	964
43	Vertically Aligned WO₃ Nanowire Arrays Grown Directly on Transparent Conducting Oxide Coated Glass: Synthesis and Photoelectrochemical Properties. Nano Letters, 2011, 11, 203-208.	4.5	550
44	Hydrothermal Synthesis of Na_{0.5}La_{0.5}TiO₃â€“LaCrO₃ Solidâ€Solution Singleâ€Crystal Nanocubes for Visibleâ€Lightâ€Driven Photocatalytic H₂ Evolution. Chemistry - A European Journal, 2011, 17, 7858-7867.	1.7	43
45	Synthesis, characterization, and photoelectrochemical study of Cd1â^'xZnxS solid solution thin films deposited by spray pyrolysis for water splitting. International Journal of Hydrogen Energy, 2010, 35, 7036-7042.	3.8	52
46	Influence of Sr-doping on the photocatalytic activities of CdSâ€“ZnS solid solution photocatalysts. International Journal of Hydrogen Energy, 2010, 35, 2048-2057.	3.8	123
47	Semiconductor-based Photocatalytic Hydrogen Generation. Chemical Reviews, 2010, 110, 6503-6570.	23.0	6,836
48	Photocatalytic H2 evolution under visible light irradiation on a novel Cd Cu Zn1â^'â^'S catalyst. Catalysis Communications, 2008, 9, 126-130.	1.6	103
49	Efficient photocatalytic H2 production under visible light irradiation over Ni doped Cd1â^'Zn S microsphere photocatalysts. Catalysis Communications, 2008, 9, 1720-1724.	1.6	116
50	A Novel Method for the Preparation of a Highly Stable and Active CdS Photocatalyst with a Special Surface Nanostructure. Journal of Physical Chemistry B, 2006, 110, 11139-11145.	1.2	431
51	Band structure-controlled solid solution of Cd1-xCd1-x ZnxSZnxS photocatalyst for hydrogen production by water splitting. International Journal of Hydrogen Energy, 2006, 31, 2018-2024.	3.8	457
52	Atomically Dispersed Janus Nickel Sites on Red Phosphorus for Photocatalytic Overall Water Splitting. Angewandte Chemie, 0, , .	1.6	2