Xin Zhou

List of Publications by Year
in descending order

65 papers	4,567 citations	236925 25 h-index	102487 66 g-index
67 all docs	67 docs citations	67 times ranked	7434 citing authors

#	Article	IF	Citations
1	Spatial separation of photogenerated electrons and holes among {010} and {110} crystal facets of BiVO4. Nature Communications, 2013, 4, 1432.	12.8	1,458
2	Surface optimization to eliminate hysteresis for record efficiency planar perovskite solar cells. Energy and Environmental Science, 2016, 9, 3071-3078.	30.8	870
3	Achieving overall water splitting using titanium dioxide-based photocatalysts of different phases. Energy and Environmental Science, 2015, 8, 2377-2382.	30.8	313
4	Effect of Metal Doping on Electronic Structure and Visible Light Absorption of SrTiO₃ and NaTaO₃ (Metal = Mn, Fe, and Co). Journal of Physical Chemistry C, 2011, 115, 8305-8311.	3.1	181
5	A Theoretical Study on the Mechanism of Photocatalytic Oxygen Evolution on BiVO₄ in Aqueous Solution. Chemistry - A European Journal, 2013, 19, 1320-1326.	3.3	161
6	Polyhedral 30â€Faceted BiVO₄ Microcrystals Predominantly Enclosed by Highâ€Index Planes Promoting Photocatalytic Waterâ€Splitting Activity. Advanced Materials, 2018, 30, 1703119.	21.0	155
7	The nature of photogenerated charge separation among different crystal facets of BiVO₄studied by density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 23503-23510.	2.8	112
8	Cu₂O/CuO photocathode with improved stability for photoelectrochemical water reduction. RSC Advances, 2015, 5, 10790-10794.	3.6	94
9	Bismuth Vacancy-Induced Efficient CO₂ Photoreduction in BiOCl Directly from Natural Air: A Progressive Step toward Photosynthesis in Nature. Nano Letters, 2021, 21, 10260-10266.	9.1	74
10	Artificial Trees for Artificial Photosynthesis: Construction of Dendrite-Structured Î±-Fe₂O₃/g-C₃N₄ Z-Scheme System for Efficient CO₂ Reduction into Solar Fuels. ACS Applied Energy Materials, 2020, 3, 6561-6572.	5.1	67
11	Few-layered ReS₂ nanosheets vertically aligned on reduced graphene oxide for superior lithium and sodium storage. Journal of Materials Chemistry A, 2018, 6, 20267-20276.	10.3	61
12	Photogenerated Intrinsic Free Carriers in Small-molecule Organic Semiconductors Visualized by Ultrafast Spectroscopy. Scientific Reports, 2015, 5, 17076.	3.3	52
13	Recent theoretical progress in the development of perovskite photovoltaic materials. Journal of Energy Chemistry, 2018, 27, 637-649.	12.9	48
14	Anderson-Type Polyoxometalate-Assisted Synthesis of Defect-Rich Doped 1T/2H-MoSe₂ Nanosheets for Efficient Seawater Splitting and Mg/Seawater Batteries. ACS Applied Materials & Interfaces, 2022, 14, 10246-10256.	8.0	45
15	Fabrication of TiO₂(B)/Anatase Heterophase Junctions at High Temperature via Stabilizing the Surface of TiO₂(B) for Enhanced Photocatalytic Activity. Journal of Physical Chemistry C, 2019, 123, 1779-1789.	3.1	43
16	Band Modulation and Interfacial Engineering to Generate Efficient Visible-Light-Induced Bifunctional Photocatalysts. ACS Sustainable Chemistry and Engineering, 2020, 8, 2919-2930.	6.7	35
17	Tailoring the electronic structure of Î²-Ga₂O₃ by non-metal doping from hybrid density functional theory calculations. Physical Chemistry Chemical Physics, 2015, 17, 5817-5825.	2.8	34
18	DFT Simulations of Water Adsorption and Activation on Lowâ€Index Î±â€Ga₂O₃ Surfaces. Chemistry - A European Journal, 2014, 20, 6915-6926.	3.3	32

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19	Photoelectrochemical Properties of CuCrO2: Characterization of Light Absorption and Photocatalytic H2 Production Performance. Catalysis Letters, 2014, 144, 1487-1493.	2.6	32
20	Trends in non-metal doping of the SrTiO₃ surface: a hybrid density functional study. Physical Chemistry Chemical Physics, 2015, 17, 21611-21621.	2.8	31
21	The mechanism of hydrogen and oxygen evolution reactionÂinÂNiâ€“NiO/Î²-Ga2O3 photocatalyst. International Journal of Hydrogen Energy, 2016, 41, 5670-5681.	7.1	27
22	A Theoretical Perspective on Charge Separation and Transfer in Metal Oxide Photocatalysts for Water Splitting. ChemCatChem, 2019, 11, 3688-3715.	3.7	27
23	Molecular design and theoretical investigation on novel porphyrin derivatives for dye-sensitized solar cells. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	26
24	Theoretical insight into the roles of cocatalysts in the Niâ€“NiO/Î²-Ga₂O₃ photocatalyst for overall water splitting. Journal of Materials Chemistry A, 2015, 3, 10309-10319.	10.3	26
25	A highly active cocatalyst-free semiconductor photocatalyst for visible-light-driven hydrogen evolution: synergistic effect of surface defects and spatial bandgap engineering. Journal of Materials Chemistry A, 2016, 4, 13803-13808.	10.3	26
26	Strong Influence of Ti Adhesion Layer on Electronâ€“Phonon Relaxation in Thin Gold Films: Ab Initio Nonadiabatic Molecular Dynamics. ACS Applied Materials & Interfaces, 2017, 9, 43343-43351.	8.0	25
27	Shape and composition control of Bi₁₉S₂₇(Br_{3â^'x},I_x) alloyed nanowires: the role of metal ions. Chemical Science, 2015, 6, 4615-4622.	7.4	24
28	Density Functional Studies on Layered Perovskite Oxyhalide Bi₄MO₈X Photocatalysts (M = Nb and Ta, X = Cl, Br, and I). Journal of Physical Chemistry C, 2017, 121, 20662-20672.	3.1	24
29	A Yin-Yang hybrid co-catalyst (CoOx-Mo2N) for photocatalytic overall water splitting. Applied Catalysis B: Environmental, 2021, 298, 120491.	20.2	22
30	A non-fullerene acceptor with all â€œAâ€•units realizing high open-circuit voltage solution-processed organic photovoltaics. Journal of Materials Chemistry A, 2014, 2, 2657.	10.3	21
31	Temperature Dependence of Electronâ€“Phonon Interactions in Gold Films Rationalized by Time-Domain Ab Initio Analysis. Journal of Physical Chemistry C, 2017, 121, 17488-17497.	3.1	21
32	Hybrid density functional theory description of non-metal doping in perovskite BaTiO3 for visible-light photocatalysis. Journal of Solid State Chemistry, 2019, 280, 121018.	2.9	21
33	Chemical Versatility of [FeFe]-Hydrogenase Models: Distinctive Activity of [Î¼-C6H4-1,2-(Îº2-S)2][Fe2(CO)6] for Electrocatalytic CO2Reduction. ACS Catalysis, 2019, 9, 768-774.	11.2	21
34	Hot Electron Thermoreflectance Coefficient of Gold during Electronâ€“Phonon Nonequilibrium. ACS Photonics, 2018, 5, 4880-4887.	6.6	20
35	Theoretical Study of Structure, Stability, and the Hydrolysis Reactions of Small Iridium Oxide Nanoclusters. Journal of Physical Chemistry A, 2012, 116, 9985-9995.	2.5	19
36	Exploring the mechanism of water-splitting reaction in NiO_x/Î²-Ga₂O₃ photocatalysts by first-principles calculations. Physical Chemistry Chemical Physics, 2016, 18, 11111-11119.	2.8	17

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37	Theoretical investigation on RuO2 nanoclusters adsorbed on TiO2 rutile (110) and anatase (101) surfaces. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	15
38	Exsolution of Iron Oxide on LaFeO₃ Perovskite: A Robust Heterostructured Support for Constructing Self-Adjustable Pt-Based Room-Temperature CO Oxidation Catalysts. ACS Applied Materials & Interfaces, 2021, 13, 27029-27040.	8.0	15
39	Theoretical insight into the distinct photocatalytic activity between NiOx and CoOx loaded Ta3N5 photocatalyst. Applied Surface Science, 2017, 405, 289-297.	6.1	14
40	Thin Ti adhesion layer breaks bottleneck to hot hole relaxation in Au films. Journal of Chemical Physics, 2019, 150, 184701.	3.0	14
41	Origin of highly efficient photocatalyst NiO/SrTiO3 for overall water splitting: Insights from density functional theory calculations. Journal of Solid State Chemistry, 2020, 292, 121683.	2.9	14
42	Combining Lindblad Master Equation and Surface Hopping to Evolve Distributions of Quantum Particles. Journal of Physical Chemistry B, 2020, 124, 4326-4337.	2.6	13
43	Theoretical insights into the origin of highly efficient photocatalyst NiO/NaTaO3 for overall water splitting. International Journal of Hydrogen Energy, 2020, 45, 19357-19369.	7.1	13
44	Quasi-vertical Îµ-Ga2O3 solar-blind photodetectors grown on p-Si substrates with Al2O3 buffer layer by metalorganic chemical vapor deposition. Vacuum, 2022, 200, 111019.	3.5	13
45	Theoretical study of metal-doped Î²-Ga2O3 photocatalysts for overall water splitting. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	12
46	Theoretical insights into interfacial and electronic structures of NiO /SrTiO3 photocatalyst for overall water splitting. Journal of Energy Chemistry, 2019, 33, 138-148.	12.9	12
47	First-principles investigation of Î²-Ge3N4 loaded with RuO2 cocatalyst for photocatalytic overall water splitting. Journal of Energy Chemistry, 2020, 44, 24-32.	12.9	11
48	Tuning the electronic structure of BaTiO₃ for an enhanced photocatalytic performance using cationâ€“anion codoping: a first-principles study. New Journal of Chemistry, 2021, 45, 8228-8239.	2.8	11
49	Unraveling the Mechanism of Photocatalytic Water Splitting in Î±-Ga₂O₃ Loaded with a Nickel Oxide Cocatalyst: A First-Principles Investigation. Journal of Physical Chemistry C, 2019, 123, 8990-9000.	3.1	10
50	Highly Enantioselective Reactions of Cyclohexanone and Î²,Î³â€Unsaturated Î±â€Keto Ester: The Tuning of Chemoâ€selectivities by Secondary and Primary Amine Catalysts. Chinese Journal of Chemistry, 2014, 32, 985-990.	4.9	9
51	Electronâ€“Phonon Relaxation at Au/Ti Interfaces Is Robust to Alloying: Ab Initio Nonadiabatic Molecular Dynamics. Journal of Physical Chemistry C, 2019, 123, 22842-22850.	3.1	9
52	Effects of Adsorbing Noble Metal Single Atoms on the Electronic Structure and Photocatalytic Activity of Ta₃N₅. Journal of Physical Chemistry C, 2021, 125, 17600-17611.	3.1	9
53	Effects of a Ni cocatalyst on the photocatalytic hydrogen evolution reaction of anatase TiO₂ by first-principles calculations. New Journal of Chemistry, 2020, 44, 5428-5437.	2.8	8
54	Photoinduced Generation of Metastable Sulfur Vacancies Enhancing the Intrinsic Hydrogen Evolution Behavior of Semiconductors. Solar Rrl, 2021, 5, 2100580.	5.8	8

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55	Impact of non-metal dopants on band-gap engineering and photocatalytic ability of Î»-Ta2O5 from a hybrid density functional study. Journal of Alloys and Compounds, 2017, 700, 1-11.	5.5	7
56	Theoretical Investigation on Structures, Stabilities, and Hydrolysis Reactions of Small RuO₂ Nanoclusters. Chinese Journal of Chemistry, 2014, 32, 527-537.	4.9	5
57	Molecular Photophysics under Shock Compression: Ab Initio Nonadiabatic Molecular Dynamics of Rhodamine Dye. Journal of Physical Chemistry C, 2018, 122, 13600-13607.	3.1	4
58	Theoretical investigation of loading Ni clusters on the Î±-Ga2O3 surfaces for photocatalytic hydrogen evolution. Journal of Energy Chemistry, 2019, 30, 8-18.	12.9	4
59	Exploring the mechanism of Ta3N5/KTaO3 photocatalyst for overall water splitting by first-principles calculations. Journal of Energy Chemistry, 2021, 56, 353-364.	12.9	4
60	Preparation of deep eutectic solvent/graphene composite materials and their removal from fuel organic sulfide performance research. New Journal of Chemistry, 2021, 45, 15637-15646.	2.8	4
61	A theoretical study on tetragonal BaTiO3 modified by surface co-doping for photocatalytic overall water splitting. International Journal of Hydrogen Energy, 2022, 47, 19073-19085.	7.1	4
62	First-principles calculation of chalcogen-doped Sr2M2O7 (M=Nb and Ta) for visible light photocatalysis. Journal of Solid State Chemistry, 2022, 308, 122905.	2.9	2
63	Theoretical Insights into the Structure, Stability, Electronic, and Photocatalytic Properties of BaNbO₂N Low-Index Surfaces. Journal of Physical Chemistry C, 2022, 126, 6934-6946.	3.1	1
64	First-principles calculations of the structural, energetic, electronic, optical, and photocatalytic properties of BaTaO₂N low-index surfaces. New Journal of Chemistry, 2022, 46, 11540-11552.	2.8	1
65	Can 2-pyrone derivative act as an effective Ï€-linker for dye-sensitized solar cells: a theoretical study?. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	0