

# Jihua Zhang

## List of Publications by Year in descending order

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70  
papers

2,651  
citations

186209

28  
h-index

197736

49  
g-index

70  
all docs

70  
docs citations

70  
times ranked

2447  
citing authors

#	ARTICLE	IF	CITATIONS
1	Artificial Heterointerfaces Achieve Delicate Reaction Kinetics towards Hydrogen Evolution and Hydrazine Oxidation Catalysis. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5984-5993.	7.2	234
2	Manipulating dehydrogenation kinetics through dual-doping Co <sub>3</sub> N electrode enables highly efficient hydrazine oxidation assisting self-powered H <sub>2</sub> production. <i>Nature Communications</i> , 2020, 11, 1853.	5.8	229
3	Partially exposed RuP <sub>2</sub> surface in hybrid structure endows its bifunctionality for hydrazine oxidation and hydrogen evolution catalysis. <i>Science Advances</i> , 2020, 6, .	4.7	168
4	Enhanced visible-light photocatalytic activity of a g-C <sub>3</sub> N <sub>4</sub> /BiVO <sub>4</sub> nanocomposite: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10218-10226.	1.3	157
5	Cell Environment-Differentiated Self-Assembly of Nanofibers. <i>Journal of the American Chemical Society</i> , 2016, 138, 11128-11131.	6.6	155
6	Realizing the Synergy of Interface Engineering and Chemical Substitution for Ni <sub>3</sub> N Enables its Bifunctionality Toward Hydrazine Oxidation Assisted Energy-Saving Hydrogen Production. <i>Advanced Functional Materials</i> , 2021, 31, 2103673.	7.8	99
7	Dual-doped carbon hollow nanospheres achieve boosted pseudocapacitive energy storage for aqueous zinc ion hybrid capacitors. <i>Energy Storage Materials</i> , 2021, 42, 705-714.	9.5	96
8	Unusual Site-Selective Doping in Layered Cathode Strengthens Electrostatic Cohesion of Alkali-Metal Layer for Practicable Sodium-Ion Full Cell. <i>Advanced Materials</i> , 2022, 34, e2103210.	11.1	90
9	Dual Nanoislands on Ni/C Hybrid Nanosheet Activate Superior Hydrazine Oxidation-Assisted High-Efficiency H <sub>2</sub> Production. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	74
10	Realizing synergistic effect of electronic modulation and nanostructure engineering over graphitic carbon nitride for highly efficient visible-light H <sub>2</sub> production coupled with benzyl alcohol oxidation. <i>Applied Catalysis B: Environmental</i> , 2020, 269, 118772.	10.8	66
11	Engineering Electronic Transfer Dynamics and Ion Adsorption Capability in Dual-Doped Carbon for High-Energy Potassium Ion Hybrid Capacitors. <i>ACS Nano</i> , 2022, 16, 6255-6265.	7.3	65
12	Modulating charge transfer dynamics for g-C <sub>3</sub> N <sub>4</sub> through a dimension and interface engineered transition metal phosphide co-catalyst for efficient visible-light photocatalytic hydrogen generation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 6939-6945.	5.2	64
13	Magic hybrid structure as multifunctional electrocatalyst surpassing benchmark Pt/C enables practical hydrazine fuel cell integrated with energy-saving H <sub>2</sub> production. <i>EScience</i> , 2022, 2, 416-427.	25.0	57
14	Dual effects of lone-pair electrons and rattling atoms in $\text{CuBiS}_2$ on its ultralow thermal conductivity. <i>Physical Review B</i> , 2017, 96, .	1.1	52
15	Hybrid density functional study on the mechanism for the enhanced photocatalytic properties of the ultrathin hybrid layered nanocomposite g-C <sub>3</sub> N <sub>4</sub> /BiOCl. <i>Applied Surface Science</i> , 2018, 435, 1351-1360.	3.1	50
16	Revealing the structural, electronic and optical properties of lead-free perovskite derivatives of Rb <sub>2</sub> SnX <sub>6</sub> (X = Cl, Br and I): A theory calculation. <i>Solar Energy</i> , 2019, 190, 272-277.	2.9	50
17	Transition Metal and N Doping on AlP Monolayers for Bifunctional Oxygen Electrocatalysts: Density Functional Theory Study Assisted by Machine Learning Description. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 1249-1259.	4.0	48
18	Combination of Magnetic and Enhanced Mechanical Properties for Copolymer-Grafted Magnetite Composite Thermoplastic Elastomers. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 10563-10575.	4.0	47

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19	Vanadium Substitution Steering Reaction Kinetics Acceleration for Ni <sub>3</sub> N Nanosheets Endows Exceptionally Energy-Saving Hydrogen Evolution Coupled with Hydrazine Oxidation. ACS Applied Materials & Interfaces, 2021, 13, 3881-3890.	4.0	46
20	Effects of Mo/W codoping on the visible-light photocatalytic activity of monoclinic BiVO <sub>4</sub> within the GGA + U framework. RSC Advances, 2016, 6, 12290-12297.	1.7	44
21	Triblock Copolymer Elastomers with Enhanced Mechanical Properties Synthesized by RAFT Polymerization and Subsequent Quaternization through Incorporation of a Comonomer with Imidazole Groups of about 2.0 Mass Percentage. Macromolecules, 2017, 50, 6218-6226.	2.2	42
22	Artificial Heterointerfaces Achieve Delicate Reaction Kinetics towards Hydrogen Evolution and Hydrazine Oxidation Catalysis. Angewandte Chemie, 2021, 133, 6049-6058.	1.6	42
23	Single tungsten atom steered band-gap engineering for graphitic carbon nitride ultrathin nanosheets boosts visible-light photocatalytic H <sub>2</sub> evolution. Chemical Engineering Journal, 2021, 424, 130004.	6.6	39
24	Enhanced photocatalytic activities of Bi <sub>2</sub> WO <sub>6</sub> by introducing Zn to replace Bi lattice sites: a first-principles study. RSC Advances, 2015, 5, 29058-29065.	1.7	38
25	Thermoelectric optimization of $\text{AgBiS}_{1.1}$ by defect engineering for room-temperature applications. Physical Review B, 2019, 99, .		38
26	Hybrid Density Functional Theory Study of Native Defects and Nonmetal (C, N, S, and P) Doping in a Bi <sub>2</sub> WO <sub>6</sub> Photocatalyst. ACS Omega, 2020, 5, 29081-29091.	1.6	33
27	Robust, Reprocessable, and Reconfigurable Cellulose-Based Multiple Shape Memory Polymer Enabled by Dynamic Metal-Ligand Bonds. ACS Applied Materials & Interfaces, 2020, 12, 25233-25242.	4.0	32
28	General surface grafting strategy-derived carbon-modified graphitic carbon nitride with largely enhanced visible light photocatalytic H <sub>2</sub> evolution coupled with benzyl alcohol oxidation. Journal of Materials Chemistry A, 2021, 9, 7143-7149.	5.2	31
29	Sulfur incorporation modulated absorption kinetics and electron transfer behavior for nitrogen rich porous carbon nanotubes endow superior aqueous zinc ion storage capability. Journal of Materials Chemistry A, 2022, 10, 9355-9362.	5.2	31
30	Ag-Mg antisite defect induced high thermoelectric performance of $\text{Fe}_2\text{MgAgSb}$ . Scientific Reports, 2017, 7, 2572.	1.6	28
31	A graphene-coupled Bi <sub>2</sub> WO <sub>6</sub> nanocomposite with enhanced photocatalytic performance: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 14113-14121.	1.3	27
32	Phase-Selective Synthesis of Ruthenium Phosphide in Hybrid Structure Enables Efficient Hybrid Water Electrolysis Under pH-Universal Conditions. Small, 2022, 18, e2200242.	5.2	24
33	$\text{BiVO}_4$ - $\text{C}$ . Physical Review Applied, 2017, 7, 044002.	1.5	23
34	Origin of high thermoelectric performance of $\text{FeNb}_{1-x}\text{Zr}_x\text{Hf}_x\text{Sb}_1-y\text{Sny}$ alloys: A first-principles study. Scientific Reports, 2016, 6, 33120.	1.6	20
35	Synthesis, order-to-disorder transition, microphase morphology and mechanical properties of BAB triblock copolymer elastomers with hard middle block and soft outer blocks. Polymer Chemistry, 2018, 9, 3067-3079.	1.9	18
36	The n-type and p-type conductivity mechanisms of the bulk BiOCl photocatalyst from hybrid density functional theory calculations. Physical Chemistry Chemical Physics, 2021, 23, 19841-19853.	1.3	18

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37	First-principles study of Ga-vacancy induced magnetism in $\hat{\Gamma}^2$ -Ga <sub>2</sub> O <sub>3</sub> . Physical Chemistry Chemical Physics, 2017, 19, 28928-28935.	1.3	17
38	ZIF-8@polyoxometalate derived Si-doped ZnWO <sub>4</sub> @ZnO nanocapsules with open-shaped structures for efficient visible light photocatalysis. Chemical Communications, 2018, 54, 13786-13789.	2.2	17
39	Effects of native defects and cerium impurity on the monoclinic BiVO <sub>4</sub> photocatalyst obtained via PBE+U calculations. Physical Chemistry Chemical Physics, 2020, 22, 25297-25305.	1.3	17
40	Strain engineering in single-atom catalysts: GaPS <sub>4</sub> for bifunctional oxygen reduction and evolution. Inorganic Chemistry Frontiers, 2022, 9, 4272-4280.	3.0	15
41	Infrared, visible and ultraviolet absorptions of transition metal doped ZnS crystals with spin-polarized bands. Journal of Solid State Chemistry, 2011, 184, 477-480.	1.4	14
42	Fabrication of Copolymer-Grafted Multiwalled Carbon Nanotube Composite Thermoplastic Elastomers Filled with Unmodified MWCNTs as Additional Nanofillers To Significantly Improve Both Electrical Conductivity and Mechanical Properties. Industrial & Engineering Chemistry Research, 2015, 54, 12597-12606.	1.8	14
43	Structural properties and strain engineering of a BeB <sub>2</sub> monolayer from first-principles. RSC Advances, 2017, 7, 38410-38414.	1.7	14
44	Effect of Cholesterol on Membrane Dipole Potential: Atomistic and Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3780-3795.	2.3	14
45	Diamond nanowires with nitrogen vacancy under a transverse electric field. Physical Review B, 2015, 91, .	1.1	11
46	Electronic structure and thermoelectric properties of the Zintl compounds Sr <sub>5</sub> Al <sub>2</sub> Sb <sub>6</sub> and Ca <sub>5</sub> Al <sub>2</sub> Sb <sub>6</sub> : first-principles study. RSC Advances, 2015, 5, 50720-50728.	1.7	10
47	An impurity intermediate band due to Pb doping induced promising thermoelectric performance of Ca <sub>5</sub> In <sub>2</sub> Sb <sub>6</sub> . Physical Chemistry Chemical Physics, 2015, 17, 15156-15164.	1.3	10
48	The Thermodynamic Stability, Electronic and Photocatalytic Properties of the ZnWO <sub>4</sub> (100) Surface as Predicted by Screened Hybrid Density Functional Theory. ACS Omega, 2021, 6, 15057-15067.	1.6	10
49	Thermodynamic stability and electronic structure properties of the Bi <sub>2</sub> WO <sub>6</sub> (0 0 1) surface: First principle calculation. Applied Surface Science, 2021, 548, 149053.	3.1	9
50	Electronic and optical properties of doped crystals: First-principles calculations. Solid State Communications, 2009, 149, 1188-1192.	0.9	8
51	Hybrid density functional studies for the effect of oxygen vacancy on the visible light photocatalytic activity in M (M=Li, Na, K, Rb, Cs)-doped $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg" \rangle \langle \text{mml:mi} \rangle \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -Bi <sub>2</sub> O <sub>3</sub> . Journal of Physics and Chemistry of Solids, 2020, 146, 109581.	1.9	8
52	A triffecta of g-C <sub>3</sub> N <sub>4</sub> : enhanced visible-spectrum absorption, increased structural distortion and boosted electronic-transfer dynamics. Chemical Communications, 2021, 57, 927-930.	2.2	8
53	Thickness Control of the Spin-Polarized Two-Dimensional Electron Gas in LaAlO <sub>3</sub> /BaTiO <sub>3</sub> Superlattices. Scientific Reports, 2018, 8, 467.	1.6	7
54	Comparative study of the binding mode between cytochrome P450 17A1 and prostate cancer drugs in the absence of haem iron. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4161-4170.	2.0	7

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55	Hybrid density functional studies of native defects and H impurities in wurtzite CdSe. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 7474-7482.	1.3	7
56	The nature of the high thermoelectric properties of CuInX <sub>2</sub> (X = S, Se and Te): First-principles study. <i>Applied Surface Science</i> , 2018, 458, 564-571.	3.1	6
57	Dual Nanoislands on Ni/C Hybrid Nanosheet Activate Superior Hydrazine Oxidation-Assisted High-Efficiency H <sub>2</sub> Production. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	6
58	Novel Z-Scheme BiOM <sub>2</sub> X <sub>2</sub> (M = Cl, Tl) ETQqO O rgBT /Overlock 10 Tf 50 632 Td (Br)/ <sup>12</sup> -Bi<sub>2</sub>S<sub>3</sub> Photocatalysts with O Vacancies: A Study on the Hybrid Density Functional Approach. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11788-11799.	1.5	6
59	First-principles study on electronic and optical properties of Cu-doped LiF with Li vacancy. <i>Physica B: Condensed Matter</i> , 2012, 407, 2458-2461.	1.3	5
60	Highly sensitive non-enzymatic glucose sensor based on CuMn <sub>2</sub> O <sub>4</sub> shuttles supporting on Ni foam. <i>Ionics</i> , 2022, 28, 2447-2456.	1.2	5
61	Structural stability and electronic properties of the new superconductor (Ca <sub>4</sub> Al <sub>2</sub> O <sub>6</sub> As <sub>2</sub> ) (Fe <sub>2</sub> As <sub>2</sub> ) from first-principles study. <i>Superconductor Science and Technology</i> , 2011, 24, 105014.	1.8	4
62	A Possible New Parent Compound Sr <sub>4</sub> Al <sub>2</sub> O <sub>6</sub> Fe <sub>2</sub> As <sub>2</sub> with High-TC Superconductivity. <i>Journal of the Physical Society of Japan</i> , 2012, 81, 024713.	0.7	4
63	Making a Rapid Completion of Crystallization for Bisphenol A Polycarbonate by a Double-Layer Film Method. <i>Industrial &amp; Engineering Chemistry Research</i> , 2018, 57, 6797-6803.	1.8	4
64	H <sub>2</sub> /g-C <sub>3</sub> N <sub>4</sub> /GO-COOH Composited by Acid-Treated g-C <sub>3</sub> N <sub>4</sub> and Functionalized Graphene Oxide for Efficient Photocatalytic H <sub>2</sub> Production. <i>Energy &amp; Fuels</i> , 2022, 36, 6005-6012.	2.5	4
65	Modulation effects of Cu doping on magnetic properties of Zn(Ni)O: First-principle calculations. <i>Journal of Magnetism and Magnetic Materials</i> , 2011, 323, 3117-3120.	1.0	3
66	The first-principles study of n-Ha <sup>6</sup> V <sub>2</sub> Sn complex: impurity effects on p-type SnO monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19275-19281.	1.3	3
67	The stability and electronic and photocatalytic properties of the ZnWO <sub>4</sub> (010) surface determined from first-principles and thermodynamic calculations. <i>RSC Advances</i> , 2021, 11, 23477-23490.	1.7	3
68	Molecular dynamics study on the stability and properties of <sup>13</sup> C-geyne. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2014, 63, 207303.	0.2	2
69	Effects of Fluorination and Molybdenum Codoping on Monoclinic BiVO <sub>4</sub> Photocatalyst by HSE Calculations. <i>ACS Omega</i> , 0, , .	1.6	2
70	Environmentally benign general synthesis of nonconsecutive carbon-coated RuP <sub>2</sub> porous microsheets as efficient bifunctional electrocatalysts under neutral conditions for energy-saving H <sub>2</sub> production in hybrid water electrolysis. <i>Catalysis Science and Technology</i> , 2022, 12, 4339-4349.	2.1	2