

# Zong-Yan Zhao

## List of Publications by Citations

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131 papers	3,965 citations	31 h-index	60 g-index
137 ext. papers	4,603 ext. citations	4.7 avg, IF	5.94 L-index

#	Paper	IF	Citations
131	Solar hydrogen generation from seawater with a modified BiVO <sub>4</sub> photoanode. <i>Energy and Environmental Science</i> , <b>2011</b> , 4, 4046	35.4	486
130	High-yield synthesis of ultrathin and uniform BiVO <sub>4</sub> square nanoplates benefitting from photocatalytic reduction of CO <sub>2</sub> into renewable hydrocarbon fuel under visible light. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2011</b> , 3, 3594-601	9.5	324
129	Electronic structure and optical properties of monoclinic clinobisvanite BiVO <sub>4</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2011</b> , 13, 4746-53	3.6	277
128	Hexahedron Prism-Anchored Octahedronal CeO <sub>2</sub> : Crystal Facet-Based Homo Junction Promoting Efficient Solar Fuel Synthesis. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 9547-50	16.4	237
127	Increasing the Oxygen Vacancy Density on the TiO <sub>2</sub> Surface by La-Doping for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 18396-18400	3.8	131
126	A Facet-Dependent Schottky-Junction Electron Shuttle in a BiVO <sub>4</sub> {010}/Au/TiO <sub>2</sub> Z-Scheme Photocatalyst for Efficient Charge Separation. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1801214	15.6	125
125	Formation energy and photoelectrochemical properties of BiVO <sub>4</sub> after doping at Bi <sup>3+</sup> or V <sup>5+</sup> sites with higher valence metal ions. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 1006-13	3.6	111
124	Structural, electronic, and optical properties of Eu-doped BiOX (X = F, Cl, Br, I): a DFT+U study. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 13001-11	5.1	97
123	Mechanism of higher photocatalytic activity of anatase TiO <sub>2</sub> doped with nitrogen under visible-light irradiation from density functional theory calculation. <i>Journal Physics D: Applied Physics</i> , <b>2008</b> , 41, 025103	10.3	95
122	Robustly photogenerating H <sub>2</sub> in water using FeP/CdS catalyst under solar irradiation. <i>Scientific Reports</i> , <b>2016</b> , 6, 19846	4.9	88
121	Density functional theory study of doping effects in monoclinic clinobisvanite BiVO <sub>4</sub> . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2010</b> , 374, 4919-4927	2.3	85
120	Effects of lanthanide doping on electronic structures and optical properties of anatase TiO <sub>2</sub> from density functional theory calculations. <i>Journal Physics D: Applied Physics</i> , <b>2008</b> , 41, 085417	3	76
119	Preparation and properties of Ce-doped TiO <sub>2</sub> photocatalyst. <i>Materials Research Bulletin</i> , <b>2012</b> , 47, 1869-1873	18.73	69
118	Luminescence properties of Sm <sup>3+</sup> -doped TiO <sub>2</sub> nanoparticles: Synthesis, characterization, and mechanism. <i>Journal of Alloys and Compounds</i> , <b>2013</b> , 554, 12-20	5.7	65
117	A Theoretical Study of Water Adsorption and Decomposition on the Low-Index Stoichiometric Anatase TiO <sub>2</sub> Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 7430-7441	3.8	60
116	In <sup>3+</sup> -doped BiVO <sub>4</sub> photoanodes with passivated surface states for photoelectrochemical water oxidation. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 10456-10465	13	57
115	BiVO <sub>4</sub> nano-leaves: Mild synthesis and improved photocatalytic activity for O <sub>2</sub> production under visible light irradiation. <i>CrystEngComm</i> , <b>2011</b> , 13, 2500	3.3	57

114	Structure and Properties of Water on the Anatase TiO <sub>2</sub> (101) Surface: From Single-Molecule Adsorption to Interface Formation. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 11054-11061	3.8	54
113	Electronic Structure and Optical Properties of BiOI Ultrathin Films for Photocatalytic Water Splitting. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 10732-7	5.1	51
112	Study of the layer-dependent properties of MoS <sub>2</sub> nanosheets with different crystal structures by DFT calculations. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 1867-1879	5.5	50
111	Polymerizable complex synthesis of BaZr <sub>1-x</sub> Sn <sub>x</sub> O <sub>3</sub> photocatalysts: Role of Sn <sup>4+</sup> in the band structure and their photocatalytic water splitting activities. <i>Journal of Materials Chemistry</i> , <b>2010</b> , 20, 6772		46
110	Ca <sub>2</sub> Al <sub>2</sub> SiO <sub>7</sub> :Bi <sup>3+</sup> , Eu <sup>3+</sup> , Tb <sup>3+</sup> : A potential single-phased tunable-color-emitting phosphor. <i>Journal of Luminescence</i> , <b>2013</b> , 135, 206-210	3.8	45
109	Structure and energetics of low-index stoichiometric monoclinic clinobisvanite BiVO <sub>4</sub> surfaces. <i>RSC Advances</i> , <b>2011</b> , 1, 874	3.7	45
108	Designed Highly Effective Photocatalyst of Anatase TiO <sub>2</sub> Codoped with Nitrogen and Vanadium Under Visible-light Irradiation Using First-principles. <i>Catalysis Letters</i> , <b>2008</b> , 124, 111-117	2.8	44
107	Novel whey protein-based aqueous polymer-isocyanate adhesive for glulam. <i>Journal of Applied Polymer Science</i> , <b>2011</b> , 120, 220-225	2.9	42
106	Surface properties and electronic structure of low-index stoichiometric anatase TiO <sub>2</sub> surfaces. <i>Journal of Physics Condensed Matter</i> , <b>2010</b> , 22, 175008	1.8	42
105	Reconstruction of the (001) surface of TiO <sub>2</sub> nanosheets induced by the fluorine-surfactant removal process under UV-irradiation for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 4763-9	3.6	37
104	Far-Red-Emitting BiOCl:Eu <sup>3+</sup> Phosphor with Excellent Broadband NUV-Excitation for White-Light-Emitting Diodes. <i>Journal of the American Ceramic Society</i> , <b>2015</b> , 98, 2170-2176	3.8	36
103	First-principles study on the doping effects of nitrogen on the electronic structure and optical properties of Cu <sub>2</sub> O. <i>RSC Advances</i> , <b>2013</b> , 3, 84-90	3.7	33
102	Fundamental properties of delafossite CuFeO <sub>2</sub> as photocatalyst for solar energy conversion. <i>Journal of Alloys and Compounds</i> , <b>2020</b> , 819, 153032	5.7	32
101	Studied Localized Surface Plasmon Resonance Effects of Au Nanoparticles on TiO <sub>2</sub> by FDTD Simulations. <i>Catalysts</i> , <b>2018</b> , 8, 236	4	31
100	Band-edge electronic structure of In <sub>2</sub> S <sub>3</sub> : the role of s or p orbitals of atoms at different lattice positions. <i>ChemPhysChem</i> , <b>2012</b> , 13, 1551-6	3.2	25
99	Electronic structure and optical properties of wurtzite-kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2013</b> , 377, 417-422	2.3	24
98	Interfacial properties of Bi <sub>2</sub> O <sub>3</sub> homo-junction from first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2015</b> , 379, 2766-2771	2.3	24
97	Series of ZnSn(OH) Polyhedra: Enhanced CO Dissociation Activation and Crystal Facet-Based Homoijunction Boosting Solar Fuel Synthesis. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 5704-5709	5.1	23

96	Photocatalytic activity of La <sup>3+</sup> -codoped NaTaO <sub>3</sub> for H <sub>2</sub> evolution from water under visible-light irradiation. <i>Journal Physics D: Applied Physics</i> , <b>2011</b> , 44, 165401	3	23
95	Understanding the interaction of water with anatase TiO <sub>2</sub> (101) surface from density functional theory calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2011</b> , 375, 2939-2943	4.3	23
94	Theoretical calculations for localized surface plasmon resonance effects of Cu/TiO <sub>2</sub> nanosphere: Generation, modulation, and application in photocatalysis. <i>Solar Energy Materials and Solar Cells</i> , <b>2020</b> , 208, 110385	6.4	23
93	Electronic Structure and Optical Properties of BiOI as a Photocatalyst Driven by Visible Light. <i>Catalysts</i> , <b>2016</b> , 6, 133	4	23
92	Structural, Electronic, and Optical Properties of BiOX <sub>1-x</sub> Y <sub>x</sub> (X, Y = F, Cl, Br, and I) Solid Solutions from DFT Calculations. <i>Scientific Reports</i> , <b>2016</b> , 6, 31449	4.9	22
91	Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO <sub>4</sub> photoanode by W <sup>6+</sup> codoping. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 16965-16974	13	22
90	Water Adsorption and Decomposition on N/V-Doped Anatase TiO <sub>2</sub> (101) Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 6172-6184	3.8	22
89	Theoretical Study of Pt Cocatalyst Loading on Anatase TiO <sub>2</sub> (101) Surface: From Surface Doping to Interface Forming. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 24591-24602	3.8	21
88	First-principles calculations on electronic structures of N/V-doped and N-V-doped anatase TiO <sub>2</sub> (101) surfaces. <i>ChemPhysChem</i> , <b>2012</b> , 13, 3836-47	3.2	21
87	The electronic structure and photoluminescence properties of BiOCl:Eu <sup>3+</sup> from first-principles calculations. <i>Journal of Luminescence</i> , <b>2014</b> , 156, 205-211	3.8	20
86	First-principles study on doping effects of sodium in kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> . <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 9235-41	5.1	20
85	Insight into insulator-to-metal transition of sulfur-doped silicon by DFT calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 17499-506	3.6	19
84	Understanding the interfacial properties of graphene-based materials/BiOI heterostructures by DFT calculations. <i>Applied Surface Science</i> , <b>2017</b> , 406, 8-20	6.7	18
83	Spontaneous Polarization Effect and Photocatalytic Activity of Layered Compound of BiOI <sub>2</sub> O. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 15344-15353	5.1	18
82	Single Water Molecule Adsorption and Decomposition on the Low-Index Stoichiometric Rutile TiO <sub>2</sub> Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 4287-4295	3.8	18
81	Defect Physics of BiOI as High Efficient Photocatalyst Driven by Visible Light. <i>Journal of the American Ceramic Society</i> , <b>2016</b> , 99, 3015-3024	3.8	17
80	Analysis of sulfur modification mechanism for anatase and rutile TiO <sub>2</sub> by different doping modes based on GGA + U calculations. <i>RSC Advances</i> , <b>2014</b> , 4, 32100	3.7	17
79	Electronic structure and optical properties of bismuth chalcogenides Bi <sub>2</sub> Q <sub>3</sub> (Q = O, S, Se, Te) by first-principles calculations. <i>Computational Materials Science</i> , <b>2018</b> , 142, 312-319	3.2	17

78	Structural and electronic properties of low-index stoichiometric BiOI surfaces. <i>Materials Chemistry and Physics</i> , <b>2017</b> , 193, 164-176	4.4	16
77	Synthesis and photoluminescence properties of MgAl(PO <sub>4</sub> )O:Eu <sup>3+</sup> red phosphor for white LEDs. <i>Ceramics International</i> , <b>2013</b> , 39, 2821-2825	5.1	16
76	The influence of alkali ions size on the superbroadband NIR emission from bismuth-doped alkali aluminoborophosphosilicate glasses. <i>Optical Materials</i> , <b>2012</b> , 35, 61-64	3.3	16
75	Effect of optical basicity on broadband infrared fluorescence in erbium-doped germanate glasses. <i>Journal of Alloys and Compounds</i> , <b>2012</b> , 513, 339-342	5.7	14
74	Construction of direct Z-scheme WO <sub>3</sub> /ZnS heterojunction to enhance the photocatalytic degradation of tetracycline antibiotic. <i>Journal of Environmental Chemical Engineering</i> , <b>2021</b> , 9, 105111	6.8	14
73	DFT calculations for single-atom confinement effects of noble metals on monolayer g-CN for photocatalytic applications.. <i>RSC Advances</i> , <b>2021</b> , 11, 4276-4285	3.7	14
72	Electronic, optical, and mechanical properties of Cu <sub>2</sub> ZnSnS <sub>4</sub> with four crystal structures. <i>Journal of Semiconductors</i> , <b>2015</b> , 36, 083004	2.3	12
71	Interfacial micro-structure and properties of TiO <sub>2</sub> /SnO <sub>2</sub> heterostructures with rutile phase: A DFT calculation investigation. <i>Applied Surface Science</i> , <b>2018</b> , 451, 258-271	6.7	12
70	Density functional theory study on the metal-support interaction between a Au cluster and an anatase TiO(001) surface. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 22069-22077	3.6	12
69	Formulation designs and characterisations of whey-protein based API adhesives. <i>Pigment and Resin Technology</i> , <b>2011</b> , 40, 410-417	1	12
68	Preparation and photocatalytic property of LiCr(WO <sub>4</sub> ) <sub>2</sub> . <i>Journal of Alloys and Compounds</i> , <b>2009</b> , 485, 346-350	5.7	12
67	DFT study on the interfacial properties of vertical and in-plane BiOI/BiOIO hetero-structures. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 9900-9911	3.6	11
66	High-Throughput Screening Delafossite CuMO <sub>2</sub> (M = IIIA, 3d, 4d, 5d, and RE) Optoelectronic Functional Materials Based on First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 14292-14302	3.8	11
65	Modification mechanism of praseodymium doping for the photocatalytic performance of TiO <sub>2</sub> : a combined experimental and theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 19087-95	3.6	11
64	Monophasic zircon-type tetragonal Eu <sub>1-x</sub> BixVO <sub>4</sub> solid-solution: synthesis, characterization, and optical properties. <i>Materials Research Bulletin</i> , <b>2014</b> , 57, 306-310	5.1	11
63	Excess oxygen in delafossite CuFeO <sub>2</sub> + $\delta$ Synthesis, characterization, and applications in solar energy conversion. <i>Chemical Engineering Journal</i> , <b>2020</b> , 396, 125290	14.7	10
62	Comparison studies of interfacial energetic and electronic properties of bimetallic AuCu/TiO <sub>2</sub> hetero-structures from DFT calculations. <i>Inorganic Chemistry Frontiers</i> , <b>2018</b> , 5, 1062-1075	6.8	10
61	Electronic structures of efficient M BiO <sub>3</sub> (M = Li, Na, K, Ag) photocatalyst. <i>Chinese Physics B</i> , <b>2016</b> , 25, 037102	1.2	10

60	Electronic structure and optical properties of Si <sub>1-x</sub> Ge <sub>x</sub> compounds with different crystal structures. <i>RSC Advances</i> , <b>2014</b> , 4, 36485-36493	3.7	10
59	Density functional theory study the effects of point defects in In <sub>2</sub> S <sub>3</sub> . <i>Computational Materials Science</i> , <b>2013</b> , 73, 139-145	3.2	10
58	Unraveling the role of cuprous oxide and boosting solar energy conversion via interface engineering in a Cu/TiO <sub>2</sub> plasmonic photocatalyst. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 8567-8578	7.1	9
57	Analysis of the electronic structures of 3d transition metals doped CuGaS <sub>2</sub> based on DFT calculations. <i>Journal of Semiconductors</i> , <b>2014</b> , 35, 013002	2.3	9
56	WATER-RESISTANT WHEY PROTEIN BASED WOOD ADHESIVE MODIFIED BY POST-TREATED PHENOL-FORMALDEHYDE OLIGOMERS (PFO). <i>BioResources</i> , <b>2012</b> , 7,	1.3	9
55	Rapid Hydroxyl Radical Generation on (001)-Facet-Exposed Ultrathin Anatase TiO <sub>2</sub> Nanosheets for Enhanced Photocatalytic Lignocellulose-to-H <sub>2</sub> Conversion. <i>ACS Catalysis</i> , <b>2022</b> , 12, 2118-2125	13.1	9
54	Effects of the Preparation Process on the Photocatalytic Performance of Delafossite CuCrO. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 16679-16689	5.1	9
53	Mildly regulated intrinsic faradaic layer at the oxide/water interface for improved photoelectrochemical performance. <i>Chemical Science</i> , <b>2020</b> , 11, 6297-6304	9.4	8
52	Interfacial properties and band alignment of noble-metal/anatase TiO <sub>2</sub> (1 0 1) hetero-structures. <i>Computational Materials Science</i> , <b>2018</b> , 151, 160-173	3.2	8
51	Effects of non-stoichiometry on electronic structure of Cu <sub>x</sub> S <sub>y</sub> compounds studied by first-principle calculations. <i>Materials Research Express</i> , <b>2019</b> , 6, 105513	1.7	8
50	Study on the effect of apatite structure on spectroscopic properties of bismuth activated alkaline earth metal chlorophosphate [M <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl; M = Ca, Sr and Ba]. <i>Materials Chemistry and Physics</i> , <b>2013</b> , 139, 220-224	4.4	8
49	Role of the Polar Electric Field in Bismuth Oxyhalides for Photocatalytic Water Splitting. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 8461-8474	5.1	8
48	Adsorption of Au <sub>x</sub> Cu <sub>y</sub> (x + y = 1, 2, 3) nanoclusters on the anatase TiO <sub>2</sub> (101) surface and their catalytic activity: a density functional theory study. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 5709-5722	5.5	7
47	Investigation of energy band alignments and interfacial properties of rutile NMO/TiO (NM = Ru, Rh, Os, and Ir) by first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 29583-29593	3.6	7
46	DFT calculations study of structural, electronic, and optical properties of Cu <sub>2</sub> ZnSn(S <sub>1-x</sub> Se <sub>x</sub> ) <sub>4</sub> alloys. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 618, 248-253	5.7	7
45	Effects of Nonmetal Doping on Electronic Structures and Optical Property of Anatase TiO <sub>2</sub> from First-Principles Calculations. <i>Rare Metal Materials and Engineering</i> , <b>2015</b> , 44, 1568-1574		7
44	Impact of sulfur-, tantalum-, or co-doping on the electronic structure of anatase titanium dioxide: A systematic density functional theory investigation. <i>Materials Science in Semiconductor Processing</i> , <b>2015</b> , 33, 94-102	4.3	7
43	Ultrathin nanosheet-anchored hexahedral prismatic Bi <sub>2</sub> MoO <sub>6</sub> arrays: one-step constructed and crystal facet-based homojunctions boosting photocatalytic CO <sub>2</sub> reduction and N <sub>2</sub> fixation. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 7045-7050	5.5	7



42	Interfacial structure and properties of TiO <sub>2</sub> phase junction studied by DFT calculations. <i>Applied Surface Science</i> , <b>2019</b> , 485, 8-21	6.7	6
41	Delafossite CuGaO <sub>2</sub> as promising visible-light-driven photocatalyst: synthesis, properties, and performances. <i>Journal Physics D: Applied Physics</i> , <b>2020</b> , 53, 135102	3	6
40	Structural and electronic properties of Cu <sub>2</sub> Q and CuQ (Q = O, S, Se, and Te) studied by first-principles calculations. <i>Materials Research Express</i> , <b>2018</b> , 5, 016305	1.7	6
39	DFT study on microstructures and electronic structures of Pt mono-/bi-doped anatase TiO <sub>2</sub> (101) surface. <i>RSC Advances</i> , <b>2015</b> , 5, 17984-17992	3.7	5
38	Effects of crystal structure and composition on the photocatalytic performance of Ta-O-N functional materials. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 12005-12015	3.6	5
37	Significantly enhanced superbroadband NIR emission in bismuth-doped calcium aluminophosphosilicate glasses by PbO substitution. <i>Materials Research Bulletin</i> , <b>2013</b> , 48, 260-263	5.1	5
36	Stable structure and electronic properties of Ru <sub>1-x</sub> Ti <sub>x</sub> O <sub>2</sub> rutile type solid solutions from DFT calculations. <i>Journal of the American Ceramic Society</i> , <b>2019</b> , 102, 4976-4989	3.8	4
35	Properties of phase transition and interfaces of Cu <sub>2</sub> ZnSnS <sub>4</sub> with hetero-phase junctions. <i>Applied Surface Science</i> , <b>2019</b> , 481, 1044-1052	6.7	4
34	Synergistic effects of nonmetal co-doping with sulfur in anatase TiO <sub>2</sub> : a DFT + U study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 3426-34	3.6	4
33	Systematic studies on Yb Bi VO:Tm solid solutions: experiments and DFT calculations on up-conversion photoluminescence properties.. <i>RSC Advances</i> , <b>2018</b> , 8, 596-605	3.7	4
32	Structural and electronic properties of low-index stoichiometric Cu <sub>2</sub> ZnSnS <sub>4</sub> surfaces. <i>Materials Research Express</i> , <b>2018</b> , 5, 055902	1.7	4
31	Electronic structures of halogen-doped Cu <sub>2</sub> O based on DFT calculations. <i>Chinese Physics B</i> , <b>2014</b> , 23, 017401	1.2	4
30	Pedestrian Tracking Based on Camshift with Kalman Prediction for Autonomous Vehicles. <i>International Journal of Advanced Robotic Systems</i> , <b>2016</b> , 13, 120	1.4	4
29	Interfacial properties of g-C <sub>3</sub> N <sub>4</sub> /TiO <sub>2</sub> heterostructures studied by DFT calculations. <i>Chinese Physics B</i> , <b>2021</b> , 30, 017101	1.2	4
28	Electronic structure and optical properties of B/P-doped amorphous Si calculated by first-principles. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 638, 59-66	5.7	3
27	Regulating effect on photocatalytic water splitting performance of g-C <sub>3</sub> N <sub>4</sub> via confinement of single atom Pt based on energy band engineering: A first principles investigation. <i>Applied Surface Science</i> , <b>2021</b> , 577, 151916	6.7	3
26	Study of Ag precipitation and mechanical properties of Ti-Ta-Ag ternary alloy.. <i>RSC Advances</i> , <b>2021</b> , 11, 2976-2984	3.7	3
25	Effects of Modulation P-Doping on Thermal Stability of InAs/GaAs Quantum Dot Superluminescent Diodes. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2018</b> , 18, 7536-7541	1.3	3

24	A High-Throughput Study of the Electronic Structure and Physical Properties of Short-Period (GaAs)(AlAs) (m, n $\neq$ 0) Superlattices Based on Density Functional Theory Calculations. <i>Nanomaterials</i> , <b>2018</b> , 8,	5.4	3
23	Mechanistic insight into the dispersion behavior of single platinum atom on monolayer g-C <sub>3</sub> N <sub>4</sub> in single-atom catalysts from density functional theory calculations. <i>Applied Surface Science</i> , <b>2021</b> , 566, 150697	6.7	3
22	Interfacial interaction and effects of GaAs/Graphene hetero-structures studied by First-principle calculations. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 795, 351-360	5.7	2
21	The effects of localized surface plasmon resonance on Cu <sub>2</sub> FeS as a full-spectrum-response photocatalyst. <i>Journal Physics D: Applied Physics</i> , <b>2020</b> , 53, 265103	3	2
20	Interfacial properties of Cu <sub>7</sub> S <sub>4</sub> /MnS heterostructure from first-principles calculations. <i>Journal of Physics and Chemistry of Solids</i> , <b>2019</b> , 134, 141-148	3.9	2
19	Alpha-NaYF <sub>4</sub> :Nd <sup>3+</sup> nanocrystal with near-infrared to near-infrared luminescence for bioimaging applications. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2014</b> , 14, 3910-3	1.3	2
18	Electronic structure of O-doped SiGe calculated by DFT + U method. <i>Chinese Physics B</i> , <b>2016</b> , 25, 127101	1.2	2
17	Theoretical study of CO oxidation on Au <sub>1</sub> /Co <sub>3</sub> O <sub>4</sub> (110) single atom catalyst using density functional theory calculations. <i>Materials Science in Semiconductor Processing</i> , <b>2021</b> , 123, 105578	4.3	2
16	Analysis of electronic structure and optical properties of N-doped SiO <sub>2</sub> based on DFT calculations. <i>Modern Physics Letters B</i> , <b>2015</b> , 29, 1550100	1.6	1
15	Hydrothermal Synthesis Nano FAP : Nd <sup>3+</sup> as Biological Probe with Near-Infrared to Near-Infrared Luminescence <b>2012</b> ,		1
14	Secondary phases in Cu <sub>2</sub> ZnSnS <sub>4</sub> thin film solar cell: The role of interfaces. <i>Physica B: Condensed Matter</i> , <b>2022</b> , 626, 413539	2.8	1
13	Assessing the Possibilities of NM <sub>x</sub> (Sb <sub>2</sub> Te <sub>3</sub> ) <sub>1-x</sub> Solid Solutions (NM = Noble Metal) for Phase-Change Memory Applications Using High-throughput Calculations. <i>Journal of Electronic Materials</i> , <b>2022</b> , 51, 1272	1.9	1
12	High-throughput computational screening of Sb <sub>2</sub> Te binary alloys for phase-change storage applications. <i>Journal of Materials Research and Technology</i> , <b>2021</b> , 15, 4243-4256	5.5	1
11	First-principles calculations to investigate the polymorph effects of CuAlO <sub>2</sub> . <i>Computational Materials Science</i> , <b>2022</b> , 209, 111403	3.2	1
10	Doping effects of Ru on Sb <sub>2</sub> Te and Sb <sub>2</sub> Te <sub>3</sub> as phase change materials studied by first-principles calculations. <i>Materials Today Communications</i> , <b>2022</b> , 31, 103669	2.5	1
9	Rational Design of a Two-Dimensional Janus CuFeO Single Layer as a Photocatalyst and Photoelectrode. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 10863-10873	6.4	0
8	High Power Compact Quantum Cascade Superluminescent Emitters with High Temperature Stability and Optical Beam Quality. <i>Journal of Nanoscience and Nanotechnology</i> , <b>2018</b> , 18, 7430-7434	1.3	0
7	Density Functional Theory Study on the Interfacial Properties of CuS/Bi <sub>2</sub> S <sub>3</sub> Heterostructure. <i>Physica Status Solidi (B): Basic Research</i> , <b>2010</b> , 2100268	1.3	0



6	Microstructure and Electronic Properties of Low-Index Stoichiometric CuFeO <sub>2</sub> Surfaces: DFT Calculations. <i>Journal of Electronic Materials</i> , <b>2022</b> , 51, 2316-2336	1.9	0
5	Stability and fundamental properties of Cu <sub>2</sub> O as optoelectronic functional materials.. <i>RSC Advances</i> , <b>2022</b> , 12, 3755-3762	3.7	
4	First-principles study on structural, mechanical, and electronic properties of disordered Pt <sub>1-x</sub> Ni <sub>x</sub> alloys. <i>Materials Chemistry and Physics</i> , <b>2020</b> , 254, 123132	4.4	
3	Effect of Ag alloying and trace precipitation on corrosion resistance of Ti-Ta-Ag ternary alloy. <i>Royal Society Open Science</i> , <b>2021</b> , 8, 210243	3.3	
2	The role and effects of Ru <sub>1-x</sub> Ti <sub>x</sub> O <sub>2</sub> solid solution transition layer in Ru/TiO <sub>2</sub> composite photocatalyst by DFT calculations. <i>Applied Surface Science</i> , <b>2022</b> , 593, 153405	6.7	
1	ZnO 1-x S x Solid Solution as Potential Buffer Layer Materials for Cu <sub>2</sub> ZnSnS <sub>4</sub> -Based Thin Film Solar Cells: Structural and Interfacial Properties. <i>Advanced Materials Interfaces</i> , <b>2020</b> , 3, 200376	4.6	