

Xiaotao Zu

List of Publications by Year in descending order

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93
papers

3,749
citations

136950

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133252

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96
docs citations

96
times ranked

4557
citing authors

#	ARTICLE	IF	CITATIONS
1	First-principles study of point defects in $\text{U}_{\text{3}}\text{Si}_{\text{2}}$: effects on the mechanical and electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4287-4297.	2.8	7
2	Synthesis and bader analyzed cobalt-phthalocyanine modified solar UV-blind $\text{In}_2\text{Ga}_2\text{O}_3$ quadrilateral nanorods photocatalysts for wide-visible-light driven H_2 evolution. <i>Applied Catalysis B: Environmental</i> , 2022, 307, 121149.	20.2	51
3	The origin of anomalous hydrogen occupation in high entropy alloys. <i>Journal of Materials Chemistry A</i> , 2022, 10, 7228-7237.	10.3	11
4	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4751-4761.	3.1	0
5	Exceptional Photocatalytic Activities of rGO Modified (B,N) Co-doped WO_3 , Coupled with CdSe QDs for One Photon Z-scheme System: A Joint Experimental and DFT Study. <i>Advanced Science</i> , 2022, 9, e2102530.	11.2	52
6	Stability of superconducting $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ thin films. <i>Science China: Physics, Mechanics and Astronomy</i> , 2022, 65, .	5.1	14
7	High- In_2O_3 perovskite membranes as insulators for two-dimensional transistors. <i>Nature</i> , 2022, 605, 262-267.	27.8	109
8	Insight into the growth behaviors of MoS_2 nanograins influenced by step edges and atomic structure of the substrate. <i>Nano Research</i> , 2022, 15, 7646-7654.	10.4	2
9	Thermal Transport and Mechanical Properties of Layered Oxychalcogenides LaCuOX ($\text{X} = \text{S}, \text{Se}, \text{and Te}$). <i>ACS Applied Energy Materials</i> , 2022, 5, 6943-6951.	5.1	5
10	Accelerating CO_2 reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. <i>Chemical Engineering Journal</i> , 2022, 446, 137161.	12.7	34
11	Melamine foam loaded tellurium doped MoSe_2 as polysulphide reservoir interlayer for Li^+S batteries. <i>Materials Technology</i> , 2022, 37, 2885-2892.	3.0	2
12	Defect formation and its effect on the thermodynamic properties of $\text{Pu}_2\text{Zr}_2\text{O}_7$ pyrochlore: a first-principles study. <i>Journal of the American Ceramic Society</i> , 2021, 104, 2301-2312.	3.8	2
13	Ultrahigh Oxygen Evolution Reaction Activity Achieved Using Ir Single Atoms on Amorphous CoO_x Nanosheets. <i>ACS Catalysis</i> , 2021, 11, 123-130.	11.2	138
14	Melamine Foam Derived $2\text{H}/1\text{T MoS}_2$ as Flexible Interlayer with Efficient Polysulfides Trapping and Fast Li^+ Diffusion to Stabilize Li^+S Batteries. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 6229-6240.	8.0	49
15	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. <i>Inorganic Chemistry</i> , 2021, 60, 1388-1397.	4.0	12
16	Superior Hydrogen Sorption Kinetics of $\text{Ti}_{0.2}\text{Zr}_{0.2}\text{Hf}_{0.2}\text{Nb}_{0.4}$ High-Entropy Alloy. <i>Metals</i> , 2021, 11, 470.	2.3	11
17	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. <i>Metals</i> , 2021, 11, 553.	2.3	4
18	A Comparative Study of Electron Radiation Responses of $\text{Pu}_2\text{Zr}_2\text{O}_7$ and $\text{La}_2\text{Zr}_2\text{O}_7$: An abinitio Molecular Dynamics Study. <i>Materials</i> , 2021, 14, 1516.	2.9	1

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19	Approaching Charge Separation Efficiency to Unity without Charge Recombination. Physical Review Letters, 2021, 126, 176401.	7.8	35
20	A Universal Atomic Substitution Conversion Strategy Towards Synthesis of Large-Size Ultrathin Nonlayered Two-Dimensional Materials. Nano-Micro Letters, 2021, 13, 165.	27.0	12
21	Crystal Symmetry Engineering in Epitaxial Perovskite Superlattices. Advanced Functional Materials, 2021, 31, 2106466.	14.9	7
22	Effect of Copper Doping on Electronic Structure and Optical Absorption of Cd ₃₃ Se ₃₃ Quantum Dots. Nanomaterials, 2021, 11, 2531.	4.1	5
23	Growth of High-Quality Monolayer Transition Metal Dichalcogenide Nanocrystals by Chemical Vapor Deposition and Their Photoluminescence and Electrocatalytic Properties. ACS Applied Materials & Interfaces, 2021, 13, 47962-47971.	8.0	14
24	First-principles study on the strain-mediated g-C ₃ N ₄ /blue phosphorene heterostructures for promising photocatalytic performance. Journal of Physics Condensed Matter, 2021, 33, 485703.	1.8	5
25	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. Npj Computational Materials, 2021, 7, .	8.7	62
26	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au ₆ Clusters. ACS Applied Energy Materials, 2021, 4, 12163-12176.	5.1	33
27	Realization of exchange bias control with manipulation of interfacial frustration in magnetic complex oxide heterostructures. Physical Review B, 2021, 104, .	3.2	8
28	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. ACS Applied Materials & Interfaces, 2021, 13, 58566-58575.	8.0	30
29	Electronic and nanostructure engineering of bifunctional MoS ₂ towards exceptional visible-light photocatalytic CO ₂ reduction and pollutant degradation. Journal of Hazardous Materials, 2020, 381, 120972.	12.4	90
30	Tuning catalytic performance by controlling reconstruction process in operando condition. Applied Catalysis B: Environmental, 2020, 260, 118103.	20.2	68
31	An abnormal incorporation behavior of Th in Gd ₂ Zr ₂ O ₇ : A first-principles study. Journal of the American Ceramic Society, 2020, 103, 1846-1853.	3.8	2
32	Nitrogen/oxygen co-doped carbon nanofoam derived from bamboo fungi for high-performance supercapacitors. Journal of Power Sources, 2020, 479, 228835.	7.8	41
33	Photocurrent Enhanced in UV-vis-NIR Photodetector Based on CdSe/CdTe Core/Shell Nanowire Arrays by Piezo-Phototronic Effect. ACS Photonics, 2020, 7, 1461-1467.	6.6	28
34	A review of Sb ₂ Se ₃ photovoltaic absorber materials and thin-film solar cells. Solar Energy, 2020, 201, 227-246.	6.1	243
35	One-Step Synthesis of N/S Codoped "Porous Carbon Cloth" as a Sulfur Carrier for Lithium-Sulfur Batteries. Energy Technology, 2020, 8, 2000188.	3.8	11
36	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. Inorganic Chemistry, 2020, 59, 9774-9782.	4.0	31

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37	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. <i>Nanomaterials</i> , 2020, 10, 340.	4.1	4
38	Layered LaCuOSe : A Promising Anisotropic Thermoelectric Material. <i>Physical Review Applied</i> , 2020, 13, .	3.8	80
39	Sodium-Mediated Epitaxial Growth of 2D Ultrathin Sb_2Se_3 Flakes for Broadband Photodetection. <i>Advanced Functional Materials</i> , 2020, 30, 1909849.	14.9	88
40	Photocatalytic solar fuel production and environmental remediation through experimental and DFT based research on CdSe-QDs-coupled P-doped-g-C ₃ N ₄ composites. <i>Applied Catalysis B: Environmental</i> , 2020, 270, 118867.	20.2	165
41	Promoting visible-light photocatalytic activities for carbon nitride based OD/2D/2D hybrid system: Beyond the conventional 4-electron mechanism. <i>Applied Catalysis B: Environmental</i> , 2020, 270, 118870.	20.2	107
42	High-performance asymmetric supercapacitors realized by copper cobalt sulfide crumpled nanoflower and N, F co-doped hierarchical nanoporous carbon polyhedron. <i>Journal of Power Sources</i> , 2020, 456, 228023.	7.8	58
43	Highly Conductive PDMS Composite Mechanically Enhanced with 3D-Graphene Network for High-Performance EMI Shielding Application. <i>Nanomaterials</i> , 2020, 10, 768.	4.1	16
44	Improved thermoelectric performance of bilayer $\text{Bi}_2\text{O}_2\text{Se}$ by the band convergence approach. <i>Journal of Materials Chemistry C</i> , 2019, 7, 11029-11039.	5.5	53
45	Interface engineering to enhance the oxygen evolution reaction under light irradiation. <i>Applied Physics Letters</i> , 2019, 115, 103901.	3.3	3
46	Optimizing the thermoelectric transport properties of $\text{Bi}_2\text{O}_2\text{Se}$ monolayer via biaxial strain. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15097-15105.	2.8	76
47	$\text{In}^{\pm}\text{-CsPbI}_3$ Colloidal Quantum Dots: Synthesis, Photodynamics, and Photovoltaic Applications. <i>ACS Energy Letters</i> , 2019, 4, 1308-1320.	17.4	65
48	Effect of Thickness of Molybdenum Nano-Interlayer on Cohesion between Molybdenum/Titanium Multilayer Film and Silicon Substrate. <i>Nanomaterials</i> , 2019, 9, 616.	4.1	4
49	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. <i>Nanomaterials</i> , 2019, 9, 461.	4.1	60
50	Failure mechanism of Au@Co ₉ S ₈ yolk-shell anode in Li-ion batteries unveiled by in-situ transmission electron microscopy. <i>Applied Physics Letters</i> , 2019, 114, .	3.3	30
51	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd ₂ Zr ₂ O ₇ . <i>Nanomaterials</i> , 2019, 9, 196.	4.1	5
52	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. <i>Nanomaterials</i> , 2019, 9, 248.	4.1	66
53	Design and facile synthesis of defect-rich C-MoS ₂ /rGO nanosheets for enhanced lithium-sulfur battery performance. <i>Beilstein Journal of Nanotechnology</i> , 2019, 10, 2251-2260.	2.8	11
54	Probing the Origin of Gold Dissolution and Tunneling Across Ni ₂ P Shell Using in situ Transmission Electron Microscopy. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 46947-46952.	8.0	2

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55	NbS ₂ : A Promising <i>p</i> -Type Ohmic Contact for Two-Dimensional Materials. Physical Review Applied, 2019, 12, .	3.8	36
56	NH ₃ -Sensing Mechanism Using Surface Acoustic Wave Sensor with AlO(OH) Film. Nanomaterials, 2019, 9, 1732.	4.1	14
57	⁵¹ Ray dose dependent conductivity of MoS ₂ nanomaterials at different temperatures. CrystEngComm, 2019, 21, 6830-6837.	2.6	7
58	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. Nanoscale Research Letters, 2018, 13, 301.	5.7	29
59	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. Nanoscale Research Letters, 2018, 13, 133.	5.7	13
60	Synthesis of S-Doped porous g-C ₃ N ₄ by using ionic liquids and subsequently coupled with Au-TiO ₂ for exceptional cocatalyst-free visible-light catalytic activities. Applied Catalysis B: Environmental, 2018, 237, 1082-1090.	20.2	151
61	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl ₃ and VCl ₃ sheets. Scientific Reports, 2016, 6, 19407.	3.3	76
62	First-principles study on the adsorption and dissociation of H ₂ molecules on Be(0 0 0 1) surfaces. Computational Materials Science, 2016, 117, 251-258.	3.0	6
63	Probing the Degradation Mechanism of Li ₂ MnO ₃ Cathode for Li-Ion Batteries. Chemistry of Materials, 2015, 27, 975-982.	6.7	130
64	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. Journal of Materials Chemistry C, 2015, 3, 3128-3134.	5.5	7
65	In situsynchrotron X-ray diffraction analysis of deformation behaviour in Ti–Ni-based thin films. Journal of Synchrotron Radiation, 2015, 22, 34-41.	2.4	0
66	Mechanism for hydrogen-promoted information of helium polymer in silicon carbide material: A diffusion study. Journal of Alloys and Compounds, 2015, 647, 167-171.	5.5	9
67	Evolution of Lattice Structure and Chemical Composition of the Surface Reconstruction Layer in Li _{1.2} Ni _{0.2} Mn _{0.6} O ₂ Cathode Material for Lithium Ion Batteries. Nano Letters, 2015, 15, 514-522.	9.1	261
68	Modulating the band gap of germanane nanoribbons for quantum well devices. Physical Chemistry Chemical Physics, 2014, 16, 18029.	2.8	9
69	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. Scientific Reports, 2014, 4, 5773.	3.3	8
70	Remarkable magnetism and ferromagnetic coupling in semi-sulfuretted transition-metal dichalcogenides. Physical Chemistry Chemical Physics, 2013, 15, 14202.	2.8	12
71	A New Regular Black Hole. International Journal of Theoretical Physics, 2013, 52, 1013-1019.	1.2	10
72	Massive Scalar Quasinormal Modes of Higher Dimensional Small Dilatonic Black Hole. International Journal of Theoretical Physics, 2013, 52, 1370-1378.	1.2	6

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73	Electronic structures and magnetic properties of MoS ₂ nanostructures: atomic defects, nanoholes, nanodots and antidots. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10385.	2.8	104
74	Controlling magnetism of MoS ₂ sheets by embedding transition-metal atoms and applying strain. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18464.	2.8	89
75	Electronic and optical properties of Co _x Al _{1-x} O ₄ (x = 0, 0.25, 0.5, 0.75, 1) alloys. <i>Applied Physics Letters</i> , 2012, 100, .	3.3	15
76	Strong asymmetrical doping properties of spinel CoAl ₂ O ₄ . <i>Journal of Applied Physics</i> , 2012, 111, 093723.	2.5	6
77	Electronic and optical properties of two-dimensional covalent organic frameworks. <i>Journal of Materials Chemistry</i> , 2012, 22, 16964.	6.7	41
78	Tensile Strain Switched Ferromagnetism in Layered NbS ₂ and NbSe ₂ . <i>ACS Nano</i> , 2012, 6, 9727-9736.	14.6	325
79	First-principles study of He point-defects in HCP rare-earth metals. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 827-830.	5.1	6
80	Review on the temperature memory effect in shape memory alloys. <i>International Journal of Smart and Nano Materials</i> , 2011, 2, 101-119.	4.2	29
81	Mechanical behavior of twinned SiC nanowires under combined tension-torsion and compression-torsion strain. <i>Journal of Applied Physics</i> , 2010, 108, .	2.5	10
82	Stone-Wales defects created by low energy recoils in single-walled silicon carbide nanotubes. <i>Journal of Applied Physics</i> , 2009, 106, .	2.5	15
83	The effects of carbon coating on nanoripples induced by focused ion beam. <i>Applied Physics Letters</i> , 2009, 94, 073103.	3.3	10
84	Ion Technique for Identifying Gamma Detector Candidates. <i>IEEE Transactions on Nuclear Science</i> , 2009, 56, 920-925.	2.0	3
85	FIRST-PRINCIPLES STUDY OF THE MIGRATION OF HELIUM IN TUNGSTEN. <i>International Journal of Modern Physics B</i> , 2009, 23, 2077-2082.	2.0	12
86	Direct formation of SiO ₂ /SnO ₂ composite nanoparticles with high surface area and high thermal stability by sol-gel-hydrothermal process. <i>Journal of Sol-Gel Science and Technology</i> , 2009, 49, 196-201.	2.4	12
87	Orientation and temperature dependence of the tensile behavior of GaN nanowires: an atomistic study. <i>Journal of Materials Science: Materials in Electronics</i> , 2008, 19, 863-867.	2.2	3
88	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. <i>Applied Physics Letters</i> , 2008, 92, 183116.	3.3	28
89	Atomistic simulations of the mechanical properties of silicon carbide nanowires. <i>Physical Review B</i> , 2008, 77, .	3.2	67
90	Nanomechanical behavior of single crystalline SiC nanotubes revealed by molecular dynamics simulations. <i>Journal of Applied Physics</i> , 2008, 104, 093506.	2.5	6

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91	Atomistic study of the melting behavior of single crystalline wurtzite gallium nitride nanowires. Journal of Materials Research, 2007, 22, 742-747.	2.6	7
92	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. Physical Review B, 2007, 76, .	3.2	45
93	Surface modification on nanoscale titanium dioxide by radiation: Preparation and characterization. Journal of Applied Polymer Science, 2006, 100, 3510-3518.	2.6	10