Xiaotao Zu

List of Publications by Citations

86 papers	2,236 citations	26 h-index	45 g-index
96 ext. papers	2,985 ext. citations	7.1 avg, IF	5.15 L-index

#	Paper	IF	Citations
86	Tensile strain switched ferromagnetism in layered NbS2 and NbSe2. *ACS Nano*, **2012**, 6, 9727-36	16.7	265
85	Evolution of lattice structure and chemical composition of the surface reconstruction layer in Li(1.2)Ni(0.2)Mn(0.6)O2 cathode material for lithium ion batteries. *Nano Letters*, **2015**, 15, 514-22	11.5	213
84	Probing the Degradation Mechanism of Li2MnO3 Cathode for Li-Ion Batteries. *Chemistry of Materials*, **2015**, 27, 975-982	9.6	107
83	A review of Sb2Se3 photovoltaic absorber materials and thin-film solar cells. *Solar Energy*, **2020**, 201, 227-246	6.8	105
82	Synthesis of S-Doped porous g-C3N4 by using ionic liquids and subsequently coupled with Au-TiO2 for exceptional cocatalyst-free visible-light catalytic activities. *Applied Catalysis B: Environmental*, **2018**, 237, 1082-1090	21.8	98
81	Electronic structures and magnetic properties of MoS2 nanostructures: atomic defects, nanoholes, nanodots and antidots. *Physical Chemistry Chemical Physics*, **2013**, 15, 10385-94	3.6	98
80	Photocatalytic solar fuel production and environmental remediation through experimental and DFT based research on CdSe-QDs-coupled P-doped-g-C3N4 composites. *Applied Catalysis B: Environmental*, **2020**, 270, 118867	21.8	86
79	Controlling magnetism of MoS2 sheets by embedding transition-metal atoms and applying strain. *Physical Chemistry Chemical Physics*, **2013**, 15, 18464-70	3.6	81
78	Ultrahigh Oxygen Evolution Reaction Activity Achieved Using Ir Single Atoms on Amorphous CoOx Nanosheets. *ACS Catalysis*, **2021**, 11, 123-130	13.1	62
77	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl3 and VCl3 sheets. *Scientific Reports*, **2016**, 6, 19407	4.9	60
76	Tuning catalytic performance by controlling reconstruction process in operando condition. *Applied Catalysis B: Environmental*, **2020**, 260, 118103	21.8	57
75	Sodium-Mediated Epitaxial Growth of 2D Ultrathin Sb2Se3 Flakes for Broadband Photodetection. *Advanced Functional Materials*, **2020**, 30, 1909849	15.6	55
74	Promoting visible-light photocatalytic activities for carbon nitride based 0D/2D/2D hybrid system: Beyond the conventional 4-electron mechanism. *Applied Catalysis B: Environmental*, **2020**, 270, 118870	21.8	54
73	Atomistic simulations of the mechanical properties of silicon carbide nanowires. *Physical Review B*, **2008**, 77,	3.3	54
72	CsPbI3 Colloidal Quantum Dots: Synthesis, Photodynamics, and Photovoltaic Applications. *ACS Energy Letters*, **2019**, 4, 1308-1320	20.1	52
71	Electronic and nanostructure engineering of bifunctional MoS towards exceptional visible-light photocatalytic CO reduction and pollutant degradation. *Journal of Hazardous Materials*, **2020**, 381, 120972	12.8	52
70	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. *Physical Review B*, **2007**, 76,	3.3	39

69	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. *Nanomaterials*, **2019**, 9,	5.4	39
68	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. *Nanomaterials*, **2019**, 9,	5.4	35
67	High-performance asymmetric supercapacitors realized by copper cobalt sulfide crumpled nanoflower and N, F co-doped hierarchical nanoporous carbon polyhedron. *Journal of Power Sources*, **2020**, 456, 228023	8.9	33
66	Electronic and optical properties of two-dimensional covalent organic frameworks. *Journal of Materials Chemistry*, **2012**, 22, 16964		33
65	Failure mechanism of Au@Co9S8 yolk-shell anode in Li-ion batteries unveiled by in-situ transmission electron microscopy. *Applied Physics Letters*, **2019**, 114, 113901	3.4	28
64	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. *Applied Physics Letters*, **2008**, 92, 183116	3.4	28
63	Optimizing the thermoelectric transport properties of BiOSe monolayer via biaxial strain. *Physical Chemistry Chemical Physics*, **2019**, 21, 15097-15105	3.6	27
62	NbS2: A Promising p-Type Ohmic Contact for Two-Dimensional Materials. *Physical Review Applied*, **2019**, 12,	4.3	27
61	Layered LaCuOSe: A Promising Anisotropic Thermoelectric Material. *Physical Review Applied*, **2020**, 13,	4.3	26
60	Improved thermoelectric performance of bilayer Bi2O2Se by the band convergence approach. *Journal of Materials Chemistry C*, **2019**, 7, 11029-11039	7.1	25
59	Review on the temperature memory effect in shape memory alloys. *International Journal of Smart and Nano Materials*, **2011**, 2, 101-119	3.6	21
58	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	6.3	16
57	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. *Inorganic Chemistry*, **2020**, 59, 9774-9782	5.1	16
56	Approaching Charge Separation Efficiency to Unity without Charge Recombination. *Physical Review Letters*, **2021**, 126, 176401	7.4	16
55	High-□perovskite membranes as insulators for two-dimensional transistors.. *Nature*, **2022**, 605, 262-267	50.4	16
54	Stone□Wales defects created by low energy recoils in single-walled silicon carbide nanotubes. *Journal of Applied Physics*, **2009**, 106, 084305	2.5	15
53	Electronic and optical properties of CoX2O4 (X = Al, Ga, In) alloys. *Applied Physics Letters*, **2012**, 100, 023901	3.4	14
52	Nitrogen/oxygen co-doped carbon nanofoam derived from bamboo fungi for high-performance supercapacitors. *Journal of Power Sources*, **2020**, 479, 228835	8.9	14

51	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. *Npj Computational Materials*, **2021**, 7,	10.9	14
50	Melamine Foam Derived 2H/1T MoS as Flexible Interlayer with Efficient Polysulfides Trapping and Fast Li Diffusion to Stabilize Li-S Batteries. *ACS Applied Materials & Interfaces*, **2021**, 13, 6229-6240	9.5	13
49	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	13
48	FIRST-PRINCIPLES STUDY OF THE MIGRATION OF HELIUM IN TUNGSTEN. *International Journal of Modern Physics B*, **2009**, 23, 2077-2082	1.1	11
47	Direct formation of SiO2/SnO2 composite nanoparticles with high surface area and high thermal stability by sol–gel-hydrothermal process. *Journal of Sol-Gel Science and Technology*, **2009**, 49, 196-201	2.3	11
46	Remarkable magnetism and ferromagnetic coupling in semi-sulfuretted transition-metal dichalcogenides. *Physical Chemistry Chemical Physics*, **2013**, 15, 14202-9	3.6	10
45	The effects of carbon coating on nanoripples induced by focused ion beam. *Applied Physics Letters*, **2009**, 94, 073103	3.4	10
44	Exceptional Photocatalytic Activities of rGO Modified (B,N) Co-Doped WO , Coupled with CdSe QDs for One Photon Z-Scheme System: A Joint Experimental and DFT Study. *Advanced Science*, **2021**, e2102530	13.6	10
43	Highly Conductive PDMS Composite Mechanically Enhanced with 3D-Graphene Network for High-Performance EMI Shielding Application. *Nanomaterials*, **2020**, 10,	5.4	9
42	Modulating the band gap of germanane nanoribbons for quantum well devices. *Physical Chemistry Chemical Physics*, **2014**, 16, 18029-33	3.6	9
41	Mechanical behavior of twinned SiC nanowires under combined tension-torsion and compression-torsion strain. *Journal of Applied Physics*, **2010**, 108, 013504	2.5	9
40	Surface modification on nanoscale titanium dioxide by radiation: Preparation and characterization. *Journal of Applied Polymer Science*, **2006**, 100, 3510-3518	2.9	8
39	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. *Scientific Reports*, **2014**, 4, 5773	4.9	7
38	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
37	A New Regular Black Hole. *International Journal of Theoretical Physics*, **2013**, 52, 1013-1019	1.1	7
36	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au6 Clusters. *ACS Applied Energy Materials*,	6.1	7
35	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. *Journal of Materials Chemistry C*, **2015**, 3, 3128-3134	7.1	6
34	Mechanism for hydrogen-promoted information of helium polymer in silicon carbide material: A diffusion study. *Journal of Alloys and Compounds*, **2015**, 647, 167-171	5.7	6

33	One-Step Synthesis of N/S Codoped Porous Carbon Cloth as a Sulfur Carrier for Lithium-Sulfur Batteries. *Energy Technology*, **2020**, 8, 2000188	3.5	6
32	Massive Scalar Quasinormal Modes of Higher Dimensional Small Dilatonic Black Hole. *International Journal of Theoretical Physics*, **2013**, 52, 1370-1378	1.1	6
31	First-principles study of He point-defects in HCP rare-earth metals. *Science China: Physics, Mechanics and Astronomy*, **2011**, 54, 827-830	3.6	6
30	Nanomechanical behavior of single crystalline SiC nanotubes revealed by molecular dynamics simulations. *Journal of Applied Physics*, **2008**, 104, 093506	2.5	6
29	Atomistic study of the melting behavior of single crystalline wurtzite gallium nitride nanowires. *Journal of Materials Research*, **2007**, 22, 742-747	2.5	6
28	NH-Sensing Mechanism Using Surface Acoustic Wave Sensor with AlO(OH) Film. *Nanomaterials*, **2019**, 9,	5.4	6
27	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. *Inorganic Chemistry*, **2021**, 60, 1388-1397	5.1	6
26	First-principles study on the adsorption and dissociation of H2 molecules on Be(0 0 0 1) surfaces. *Computational Materials Science*, **2016**, 117, 251-258	3.2	5
25	Synthesis and bader analyzed cobalt-phthalocyanine modified solar UV-blind Ga2O3 quadrilateral nanorods photocatalysts for wide-visible-light driven H2 evolution. *Applied Catalysis B: Environmental*, **2022**, 307, 121149	21.8	5
24	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. *ACS Applied Materials & Interfaces*, **2021**,	9.5	5
23	Design and facile synthesis of defect-rich C-MoS/rGO nanosheets for enhanced lithium-sulfur battery performance. *Beilstein Journal of Nanotechnology*, **2019**, 10, 2251-2260	3	5
22	Interface engineering to enhance the oxygen evolution reaction under light irradiation. *Applied Physics Letters*, **2019**, 115, 103901	3.4	3
21	Effect of Thickness of Molybdenum Nano-Interlayer on Cohesion between Molybdenum/Titanium Multilayer Film and Silicon Substrate. *Nanomaterials*, **2019**, 9,	5.4	3
20	Strong asymmetrical doping properties of spinel CoAl2O4. *Journal of Applied Physics*, **2012**, 111, 093723	2.5	3
19	Ion Technique for Identifying Gamma Detector Candidates. *IEEE Transactions on Nuclear Science*, **2009**, 56, 920-925	1.7	3
18	Orientation and temperature dependence of the tensile behavior of GaN nanowires: an atomistic study. *Journal of Materials Science: Materials in Electronics*, **2008**, 19, 863-867	2.1	3
17	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. *Metals*, **2021**, 11, 553	2.3	3
16	Ray dose dependent conductivity of MoS2 nanomaterials at different temperatures. *CrystEngComm*, **2019**, 21, 6830-6837	3.3	3

15	A Universal Atomic Substitution Conversion Strategy Towards Synthesis of Large-Size Ultrathin Nonlayered Two-Dimensional Materials. *Nano-Micro Letters*, **2021**, 13, 165	19.5	3
14	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	9.5	3
13	Superior Hydrogen Sorption Kinetics of Ti0.20Zr0.20Hf0.20Nb0.40 High-Entropy Alloy. *Metals*, **2021**, 11, 470	2.3	2
12	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd□Zr□□ *Nanomaterials*, **2019**, 9,	5.4	1
11	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. *Nanomaterials*, **2020**, 10,	5.4	1
10	Probing the Origin of Gold Dissolution and Tunneling Across NiP Shell Using in situ Transmission Electron Microscopy. *ACS Applied Materials & Interfaces*, **2019**, 11, 46947-46952	9.5	1
9	Effect of Copper Doping on Electronic Structure and Optical Absorption of CdSe Quantum Dots. *Nanomaterials*, **2021**, 11,	5.4	1
8	The origin of anomalous hydrogen occupation in high entropy alloys. *Journal of Materials Chemistry A*, **2022**, 10, 7228-7237	13	1
7	Accelerating CO2 reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. *Chemical Engineering Journal*, **2022**, 446, 137161	14.7	1
6	An abnormal incorporation behavior of Th in Gd2Zr2O7: A first-principles study. *Journal of the American Ceramic Society*, **2020**, 103, 1846-1853	3.8	0
5	Defect formation and its effect on the thermodynamic properties of Pu2Zr2O7 pyrochlore: a first-principles study. *Journal of the American Ceramic Society*, **2021**, 104, 2301-2312	3.8	0
4	Crystal Symmetry Engineering in Epitaxial Perovskite Superlattices. *Advanced Functional Materials*,21064666	19	0
3	Insight into the growth behaviors of MoS2 nanograms influenced by step edges and atomic structure of the substrate. *Nano Research*,1	10	0
2	In situ synchrotron X-ray diffraction analysis of deformation behaviour in Ti-Ni-based thin films. *Journal of Synchrotron Radiation*, **2015**, 22, 34-41	2.4	
1	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. *Journal of Physical Chemistry C*, **2022**, 126, 4751-4761	3.8	