

# Xiaotao Zu

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Synthesis and bader analyzed cobalt-phthalocyanine modified solar UV-blind EGa2O3 quadrilateral nanorods photocatalysts for wide-visible-light driven H2 evolution. <i>Applied Catalysis B: Environmental</i> , <b>2022</b> , 307, 121149	21.8	5
85	The origin of anomalous hydrogen occupation in high entropy alloys. <i>Journal of Materials Chemistry A</i> , <b>2022</b> , 10, 7228-7237	13	1
84	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. <i>Journal of Physical Chemistry C</i> , <b>2022</b> , 126, 4751-4761	3.8	
83	High- $\kappa$ Perovskite membranes as insulators for two-dimensional transistors.. <i>Nature</i> , <b>2022</b> , 605, 262-267	50.4	16
82	Accelerating CO2 reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. <i>Chemical Engineering Journal</i> , <b>2022</b> , 446, 137161	14.7	1
81	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> ,	9.5	5
80	Superior Hydrogen Sorption Kinetics of Ti0.20Zr0.20Hf0.20Nb0.40 High-Entropy Alloy. <i>Metals</i> , <b>2021</b> , 11, 470	2.3	2
79	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. <i>Metals</i> , <b>2021</b> , 11, 553	2.3	3
78	Approaching Charge Separation Efficiency to Unity without Charge Recombination. <i>Physical Review Letters</i> , <b>2021</b> , 126, 176401	7.4	16
77	Defect formation and its effect on the thermodynamic properties of Pu2Zr2O7 pyrochlore: a first-principles study. <i>Journal of the American Ceramic Society</i> , <b>2021</b> , 104, 2301-2312	3.8	0
76	Ultrahigh Oxygen Evolution Reaction Activity Achieved Using Ir Single Atoms on Amorphous CoOx Nanosheets. <i>ACS Catalysis</i> , <b>2021</b> , 11, 123-130	13.1	62
75	Melamine Foam Derived 2H/1T MoS as Flexible Interlayer with Efficient Polysulfides Trapping and Fast Li Diffusion to Stabilize Li-S Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 6229-6240	9.5	13
74	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 1388-1397	5.1	6
73	A Universal Atomic Substitution Conversion Strategy Towards Synthesis of Large-Size Ultrathin Nonlayered Two-Dimensional Materials. <i>Nano-Micro Letters</i> , <b>2021</b> , 13, 165	19.5	3
72	Effect of Copper Doping on Electronic Structure and Optical Absorption of CdSe Quantum Dots. <i>Nanomaterials</i> , <b>2021</b> , 11,	5.4	1
71	Growth of High-Quality Monolayer Transition Metal Dichalcogenide Nanocrystals by Chemical Vapor Deposition and Their Photoluminescence and Electrocatalytic Properties. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 47962-47971	9.5	3
70	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. <i>Npj Computational Materials</i> , <b>2021</b> , 7,	10.9	14

69	Exceptional Photocatalytic Activities of rGO Modified (B,N) Co-Doped WO <sub>3</sub> , Coupled with CdSe QDs for One Photon Z-Scheme System: A Joint Experimental and DFT Study. <i>Advanced Science</i> , <b>2021</b> , e2102530	13.6	10
68	Photocurrent Enhanced in UV-vis-NIR Photodetector Based on CdSe/CdTe Core/Shell Nanowire Arrays by Piezo-Phototronic Effect. <i>ACS Photonics</i> , <b>2020</b> , 7, 1461-1467	6.3	16
67	A review of Sb <sub>2</sub> Se <sub>3</sub> photovoltaic absorber materials and thin-film solar cells. <i>Solar Energy</i> , <b>2020</b> , 201, 227-246	6.8	105
66	One-Step Synthesis of N/S Codoped Borous Carbon Cloth as a Sulfur Carrier for Lithium-Sulfur Batteries. <i>Energy Technology</i> , <b>2020</b> , 8, 2000188	3.5	6
65	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 9774-9782	5.1	16
64	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	1
63	Layered LaCuOSe: A Promising Anisotropic Thermoelectric Material. <i>Physical Review Applied</i> , <b>2020</b> , 13,	4.3	26
62	Sodium-Mediated Epitaxial Growth of 2D Ultrathin Sb <sub>2</sub> Se <sub>3</sub> Flakes for Broadband Photodetection. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 1909849	15.6	55
61	Photocatalytic solar fuel production and environmental remediation through experimental and DFT based research on CdSe-QDs-coupled P-doped-g-C <sub>3</sub> N <sub>4</sub> composites. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 270, 118867	21.8	86
60	Promoting visible-light photocatalytic activities for carbon nitride based 0D/2D/2D hybrid system: Beyond the conventional 4-electron mechanism. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 270, 118870	21.8	54
59	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> , <b>2020</b> , 456, 228023	8.9	33
58	Highly Conductive PDMS Composite Mechanically Enhanced with 3D-Graphene Network for High-Performance EMI Shielding Application. <i>Nanomaterials</i> , <b>2020</b> , 10,	5.4	9
57	An abnormal incorporation behavior of Th in Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> : A first-principles study. <i>Journal of the American Ceramic Society</i> , <b>2020</b> , 103, 1846-1853	3.8	0
56	Nitrogen/oxygen co-doped carbon nanofoam derived from bamboo fungi for high-performance supercapacitors. <i>Journal of Power Sources</i> , <b>2020</b> , 479, 228835	8.9	14
55	Electronic and nanostructure engineering of bifunctional MoS <sub>2</sub> towards exceptional visible-light photocatalytic CO reduction and pollutant degradation. <i>Journal of Hazardous Materials</i> , <b>2020</b> , 381, 120972	12.8	52
54	Tuning catalytic performance by controlling reconstruction process in operando condition. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 260, 118103	21.8	57
53	Interface engineering to enhance the oxygen evolution reaction under light irradiation. <i>Applied Physics Letters</i> , <b>2019</b> , 115, 103901	3.4	3
52	Optimizing the thermoelectric transport properties of Bi <sub>2</sub> Se <sub>3</sub> monolayer via biaxial strain. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15097-15105	3.6	27

51	BiCsPbI <sub>3</sub> Colloidal Quantum Dots: Synthesis, Photodynamics, and Photovoltaic Applications. <i>ACS Energy Letters</i> , <b>2019</b> , 4, 1308-1320	20.1	52
50	Effect of Thickness of Molybdenum Nano-Interlayer on Cohesion between Molybdenum/Titanium Multilayer Film and Silicon Substrate. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	3
49	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	35
48	Failure mechanism of Au@Co <sub>9</sub> S <sub>8</sub> yolk-shell anode in Li-ion batteries unveiled by in-situ transmission electron microscopy. <i>Applied Physics Letters</i> , <b>2019</b> , 114, 113901	3.4	28
47	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	1
46	Improved thermoelectric performance of bilayer Bi <sub>2</sub> O <sub>2</sub> Se by the band convergence approach. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 11029-11039	7.1	25
45	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	39
44	Design and facile synthesis of defect-rich C-MoS <sub>2</sub> /rGO nanosheets for enhanced lithium-sulfur battery performance. <i>Beilstein Journal of Nanotechnology</i> , <b>2019</b> , 10, 2251-2260	3	5
43	Probing the Origin of Gold Dissolution and Tunneling Across NiP Shell Using in situ Transmission Electron Microscopy. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 46947-46952	9.5	1
42	NbS <sub>2</sub> : A Promising p-Type Ohmic Contact for Two-Dimensional Materials. <i>Physical Review Applied</i> , <b>2019</b> , 12,	4.3	27
41	NH <sub>3</sub> -Sensing Mechanism Using Surface Acoustic Wave Sensor with AlO(OH) Film. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	6
40	γ-Ray dose dependent conductivity of MoS <sub>2</sub> nanomaterials at different temperatures. <i>CrystEngComm</i> , <b>2019</b> , 21, 6830-6837	3.3	3
39	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. <i>Nanoscale Research Letters</i> , <b>2018</b> , 13, 133	5	7
38	Synthesis of S-Doped porous g-C <sub>3</sub> N <sub>4</sub> by using ionic liquids and subsequently coupled with Au-TiO <sub>2</sub> for exceptional cocatalyst-free visible-light catalytic activities. <i>Applied Catalysis B: Environmental</i> , <b>2018</b> , 237, 1082-1090	21.8	98
37	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. <i>Nanoscale Research Letters</i> , <b>2018</b> , 13, 301	5	13
36	First-principles study on the adsorption and dissociation of H <sub>2</sub> molecules on Be(0 0 0 1) surfaces. <i>Computational Materials Science</i> , <b>2016</b> , 117, 251-258	3.2	5
35	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl <sub>3</sub> and VCl <sub>3</sub> sheets. <i>Scientific Reports</i> , <b>2016</b> , 6, 19407	4.9	60
34	Probing the Degradation Mechanism of Li <sub>2</sub> MnO <sub>3</sub> Cathode for Li-Ion Batteries. <i>Chemistry of Materials</i> , <b>2015</b> , 27, 975-982	9.6	107

33	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. <i>Journal of Materials Chemistry C</i> , <b>2015</b> , 3, 3128-3134	7.1	6
32	In situ synchrotron X-ray diffraction analysis of deformation behaviour in Ti-Ni-based thin films. <i>Journal of Synchrotron Radiation</i> , <b>2015</b> , 22, 34-41	2.4	
31	Mechanism for hydrogen-promoted information of helium polymer in silicon carbide material: A diffusion study. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 647, 167-171	5.7	6
30	Evolution of lattice structure and chemical composition of the surface reconstruction layer in Li(1.2)Ni(0.2)Mn(0.6)O <sub>2</sub> cathode material for lithium ion batteries. <i>Nano Letters</i> , <b>2015</b> , 15, 514-22	11.5	213
29	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. <i>Scientific Reports</i> , <b>2014</b> , 4, 5773	4.9	7
28	Modulating the band gap of germanane nanoribbons for quantum well devices. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 18029-33	3.6	9
27	Remarkable magnetism and ferromagnetic coupling in semi-sulfuretted transition-metal dichalcogenides. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 14202-9	3.6	10
26	A New Regular Black Hole. <i>International Journal of Theoretical Physics</i> , <b>2013</b> , 52, 1013-1019	1.1	7
25	Massive Scalar Quasinormal Modes of Higher Dimensional Small Dilatonic Black Hole. <i>International Journal of Theoretical Physics</i> , <b>2013</b> , 52, 1370-1378	1.1	6
24	Electronic structures and magnetic properties of MoS <sub>2</sub> nanostructures: atomic defects, nanoholes, nanodots and antidots. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 10385-94	3.6	98
23	Controlling magnetism of MoS <sub>2</sub> sheets by embedding transition-metal atoms and applying strain. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 18464-70	3.6	81
22	Electronic and optical properties of CoX <sub>2</sub> O <sub>4</sub> (X = Al, Ga, In) alloys. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 023901	3.6	14
21	Strong asymmetrical doping properties of spinel CoAl <sub>2</sub> O <sub>4</sub> . <i>Journal of Applied Physics</i> , <b>2012</b> , 111, 093723	2.5	3
20	Electronic and optical properties of two-dimensional covalent organic frameworks. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 16964		33
19	Tensile strain switched ferromagnetism in layered NbS <sub>2</sub> and NbSe <sub>2</sub> . <i>ACS Nano</i> , <b>2012</b> , 6, 9727-36	16.7	265
18	First-principles study of He point-defects in HCP rare-earth metals. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2011</b> , 54, 827-830	3.6	6
17	Review on the temperature memory effect in shape memory alloys. <i>International Journal of Smart and Nano Materials</i> , <b>2011</b> , 2, 101-119	3.6	21
16	Mechanical behavior of twinned SiC nanowires under combined tension-torsion and compression-torsion strain. <i>Journal of Applied Physics</i> , <b>2010</b> , 108, 013504	2.5	9

15	StoneWales defects created by low energy recoils in single-walled silicon carbide nanotubes. <i>Journal of Applied Physics</i> , <b>2009</b> , 106, 084305	2.5	15
14	The effects of carbon coating on nanoripples induced by focused ion beam. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 073103	3.4	10
13	Ion Technique for Identifying Gamma Detector Candidates. <i>IEEE Transactions on Nuclear Science</i> , <b>2009</b> , 56, 920-925	1.7	3
12	FIRST-PRINCIPLES STUDY OF THE MIGRATION OF HELIUM IN TUNGSTEN. <i>International Journal of Modern Physics B</i> , <b>2009</b> , 23, 2077-2082	1.1	11
11	Direct formation of SiO <sub>2</sub> /SnO <sub>2</sub> composite nanoparticles with high surface area and high thermal stability by sol-gel-hydrothermal process. <i>Journal of Sol-Gel Science and Technology</i> , <b>2009</b> , 49, 196-201	2.3	11
10	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. <i>Applied Physics Letters</i> , <b>2008</b> , 92, 183116	3.4	28
9	Atomistic simulations of the mechanical properties of silicon carbide nanowires. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	54
8	Nanomechanical behavior of single crystalline SiC nanotubes revealed by molecular dynamics simulations. <i>Journal of Applied Physics</i> , <b>2008</b> , 104, 093506	2.5	6
7	Orientation and temperature dependence of the tensile behavior of GaN nanowires: an atomistic study. <i>Journal of Materials Science: Materials in Electronics</i> , <b>2008</b> , 19, 863-867	2.1	3
6	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	39
5	Atomistic study of the melting behavior of single crystalline wurtzite gallium nitride nanowires. <i>Journal of Materials Research</i> , <b>2007</b> , 22, 742-747	2.5	6
4	Surface modification on nanoscale titanium dioxide by radiation: Preparation and characterization. <i>Journal of Applied Polymer Science</i> , <b>2006</b> , 100, 3510-3518	2.9	8
3	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au <sub>6</sub> Clusters. <i>ACS Applied Energy Materials</i> ,	6.1	7
2	Crystal Symmetry Engineering in Epitaxial Perovskite Superlattices. <i>Advanced Functional Materials</i> , <b>2016</b> , 26, 1604666	4.5	0
1	Insight into the growth behaviors of MoS <sub>2</sub> nanograms influenced by step edges and atomic structure of the substrate. <i>Nano Research</i> , <b>2016</b> , 9, 1000-1008	10	0