

# Xiaotao Zu

## List of Publications by Year in descending order

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93  
papers

3,749  
citations

136740

32  
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133063

59  
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96  
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96  
docs citations

96  
times ranked

4557  
citing authors

#	ARTICLE	IF	CITATIONS
1	Tensile Strain Switched Ferromagnetism in Layered NbS <sub>2</sub> and NbSe <sub>2</sub> . ACS Nano, 2012, 6, 9727-9736.	7.3	325
2	Evolution of Lattice Structure and Chemical Composition of the Surface Reconstruction Layer in Li <sub>1.2</sub> Ni <sub>0.2</sub> Mn <sub>0.6</sub> O <sub>2</sub> Cathode Material for Lithium Ion Batteries. Nano Letters, 2015, 15, 514-522.	4.5	261
3	A review of Sb <sub>2</sub> Se <sub>3</sub> photovoltaic absorber materials and thin-film solar cells. Solar Energy, 2020, 201, 227-246.	2.9	243
4	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. Applied Catalysis B: Environmental, 2020, 270, 118867.	10.8	165
5	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. Applied Catalysis B: Environmental, 2018, 237, 1082-1090.	10.8	151
6	Ultrahigh Oxygen Evolution Reaction Activity Achieved Using Ir Single Atoms on Amorphous CoO <sub>x</sub> Nanosheets. ACS Catalysis, 2021, 11, 123-130.	5.5	138
7	Probing the Degradation Mechanism of Li <sub>2</sub> MnO <sub>3</sub> Cathode for Li-Ion Batteries. Chemistry of Materials, 2015, 27, 975-982.	3.2	130
8	High- $\kappa$ perovskite membranes as insulators for two-dimensional transistors. Nature, 2022, 605, 262-267.	13.7	109
9	Promoting visible-light photocatalytic activities for carbon nitride based OD/2D/2D hybrid system: Beyond the conventional 4-electron mechanism. Applied Catalysis B: Environmental, 2020, 270, 118870.	10.8	107
10	Electronic structures and magnetic properties of MoS <sub>2</sub> nanostructures: atomic defects, nanoholes, nanodots and antidots. Physical Chemistry Chemical Physics, 2013, 15, 10385.	1.3	104
11	Electronic and nanostructure engineering of bifunctional MoS <sub>2</sub> towards exceptional visible-light photocatalytic CO <sub>2</sub> reduction and pollutant degradation. Journal of Hazardous Materials, 2020, 381, 120972.	6.5	90
12	Controlling magnetism of MoS <sub>2</sub> sheets by embedding transition-metal atoms and applying strain. Physical Chemistry Chemical Physics, 2013, 15, 18464.	1.3	89
13	Sodium-Mediated Epitaxial Growth of 2D Ultrathin Sb <sub>2</sub> Se <sub>3</sub> Flakes for Broadband Photodetection. Advanced Functional Materials, 2020, 30, 1909849.	7.8	88
14	Layered $\text{LaCuSeO}$ : A Promising Anisotropic Thermoelectric Material. Physical Review Applied, 2020, 13, .	1.5	80
15	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl <sub>3</sub> and VCl <sub>3</sub> sheets. Scientific Reports, 2016, 6, 19407.	1.6	76
16	Optimizing the thermoelectric transport properties of Bi <sub>2</sub> O <sub>2</sub> Se monolayer via biaxial strain. Physical Chemistry Chemical Physics, 2019, 21, 15097-15105.	1.3	76
17	Tuning catalytic performance by controlling reconstruction process in operando condition. Applied Catalysis B: Environmental, 2020, 260, 118103.	10.8	68
18	Atomistic simulations of the mechanical properties of silicon carbide nanowires. Physical Review B, 2008, 77, .	1.1	67

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19	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. <i>Nanomaterials</i> , 2019, 9, 248.	1.9	66
20	$\text{In}^{\pm}\text{-CsPbI}_3$ Colloidal Quantum Dots: Synthesis, Photodynamics, and Photovoltaic Applications. <i>ACS Energy Letters</i> , 2019, 4, 1308-1320.	8.8	65
21	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	62
22	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. <i>Nanomaterials</i> , 2019, 9, 461.	1.9	60
23	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.	4.0	58
24	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.	2.7	53
25	Exceptional Photocatalytic Activities of rGO Modified (B,N) Co-Doped $\text{WO}_3$ , Coupled with CdSe QDs for One Photon Z-scheme System: A Joint Experimental and DFT Study. <i>Advanced Science</i> , 2022, 9, e2102530.	5.6	52
26	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 $\text{H}_2$ evolution. <i>Applied Catalysis B: Environmental</i> , 2022, 307, 121149.	10.8	51
27	Melamine Foam Derived 2H/1T $\text{MoS}_2$ as Flexible Interlayer with Efficient Polysulfides Trapping and Fast $\text{Li}^+$ Diffusion to Stabilize $\text{Li}^+\text{-S}$ Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 6229-6240.	4.0	49
28	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. <i>Physical Review B</i> , 2007, 76, .	1.1	45
29	Electronic and optical properties of two-dimensional covalent organic frameworks. <i>Journal of Materials Chemistry</i> , 2012, 22, 16964.	6.7	41
30	Nitrogen/oxygen co-doped carbon nanofoam derived from bamboo fungi for high-performance supercapacitors. <i>Journal of Power Sources</i> , 2020, 479, 228835.	4.0	41
31	$\text{NbS}_2$ : A Promising <i>p</i> -Type Ohmic Contact for Two-Dimensional Materials. <i>Physical Review Applied</i> , 2019, 12, .	1.5	36
32	Approaching Charge Separation Efficiency to Unity without Charge Recombination. <i>Physical Review Letters</i> , 2021, 126, 176401.	2.9	35
33	Accelerating CO <sub>2</sub> reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. <i>Chemical Engineering Journal</i> , 2022, 446, 137161.	6.6	34
34	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral $\text{Au}_6$ Clusters. <i>ACS Applied Energy Materials</i> , 2021, 4, 12163-12176.	2.5	33
35	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. <i>Inorganic Chemistry</i> , 2020, 59, 9774-9782.	1.9	31
36	Failure mechanism of Au@Co <sub>9</sub> S <sub>8</sub> yolk-shell anode in Li-ion batteries unveiled by <i>in-situ</i> transmission electron microscopy. <i>Applied Physics Letters</i> , 2019, 114, .	1.5	30

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37	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. ACS Applied Materials & Interfaces, 2021, 13, 58566-58575.	4.0	30
38	Review on the temperature memory effect in shape memory alloys. International Journal of Smart and Nano Materials, 2011, 2, 101-119.	2.0	29
39	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.	3.1	29
40	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. Applied Physics Letters, 2008, 92, 183116.	1.5	28
41	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.	3.2	28
42	Highly Conductive PDMS Composite Mechanically Enhanced with 3D-Graphene Network for High-Performance EMI Shielding Application. Nanomaterials, 2020, 10, 768.	1.9	16
43	Stone-Å Wales defects created by low energy recoils in single-walled silicon carbide nanotubes. Journal of Applied Physics, 2009, 106, .	1.1	15
44	Electronic and optical properties of Co <sub>2</sub> O <sub>4</sub> (x = Al, Ga, In) alloys. Applied Physics Letters, 2012, 100, .	1.5	15
45	NH <sub>3</sub> -Sensing Mechanism Using Surface Acoustic Wave Sensor with AlO(OH) Film. Nanomaterials, 2019, 9, 1732.	1.9	14
46	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.	4.0	14
47	Stability of superconducting Nd <sub>0.8</sub> Sr <sub>0.2</sub> NiO <sub>2</sub> thin films. Science China: Physics, Mechanics and Astronomy, 2022, 65, .	2.0	14
48	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. Nanoscale Research Letters, 2018, 13, 133.	3.1	13
49	FIRST-PRINCIPLES STUDY OF THE MIGRATION OF HELIUM IN TUNGSTEN. International Journal of Modern Physics B, 2009, 23, 2077-2082.	1.0	12
50	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. Journal of Sol-Gel Science and Technology, 2009, 49, 196-201.	1.1	12
51	Remarkable magnetism and ferromagnetic coupling in semi-sulfuretted transition-metal dichalcogenides. Physical Chemistry Chemical Physics, 2013, 15, 14202.	1.3	12
52	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. Inorganic Chemistry, 2021, 60, 1388-1397.	1.9	12
53	A Universal Atomic Substitution Conversion Strategy Towards Synthesis of Large-Size Ultrathin Nonlayered Two-Dimensional Materials. Nano-Micro Letters, 2021, 13, 165.	14.4	12
54	Design and facile synthesis of defect-rich C-MoS <sub>2</sub> /rGO nanosheets for enhanced lithium-sulfur battery performance. Beilstein Journal of Nanotechnology, 2019, 10, 2251-2260.	1.5	11

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55	One-Step Synthesis of N/S Codoped Porous Carbon Cloth as a Sulfur Carrier for Lithium-Sulfur Batteries. <i>Energy Technology</i> , 2020, 8, 2000188.	1.8	11
56	Superior Hydrogen Sorption Kinetics of Ti <sub>0.2</sub> Zr <sub>0.2</sub> Hf <sub>0.2</sub> Nb <sub>0.4</sub> High-Entropy Alloy. <i>Metals</i> , 2021, 11, 470.	1.0	11
57	The origin of anomalous hydrogen occupation in high entropy alloys. <i>Journal of Materials Chemistry A</i> , 2022, 10, 7228-7237.	5.2	11
58	Surface modification on nanoscale titanium dioxide by radiation: Preparation and characterization. <i>Journal of Applied Polymer Science</i> , 2006, 100, 3510-3518.	1.3	10
59	The effects of carbon coating on nanoripples induced by focused ion beam. <i>Applied Physics Letters</i> , 2009, 94, 073103.	1.5	10
60	Mechanical behavior of twinned SiC nanowires under combined tension-torsion and compression-torsion strain. <i>Journal of Applied Physics</i> , 2010, 108, .	1.1	10
61	A New Regular Black Hole. <i>International Journal of Theoretical Physics</i> , 2013, 52, 1013-1019.	0.5	10
62	Modulating the band gap of germanane nanoribbons for quantum well devices. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 18029.	1.3	9
63	Mechanism for hydrogen-promoted information of helium polymer in silicon carbide material: A diffusion study. <i>Journal of Alloys and Compounds</i> , 2015, 647, 167-171.	2.8	9
64	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. <i>Scientific Reports</i> , 2014, 4, 5773.	1.6	8
65	Realization of exchange bias control with manipulation of interfacial frustration in magnetic complex oxide heterostructures. <i>Physical Review B</i> , 2021, 104, .	1.1	8
66	Atomistic study of the melting behavior of single crystalline wurtzite gallium nitride nanowires. <i>Journal of Materials Research</i> , 2007, 22, 742-747.	1.2	7
67	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. <i>Journal of Materials Chemistry C</i> , 2015, 3, 3128-3134.	2.7	7
68	$\beta$ -Ray dose dependent conductivity of MoS <sub>2</sub> nanomaterials at different temperatures. <i>CrystEngComm</i> , 2019, 21, 6830-6837.	1.3	7
69	Crystal Symmetry Engineering in Epitaxial Perovskite Superlattices. <i>Advanced Functional Materials</i> , 2021, 31, 2106466.	7.8	7
70	First-principles study of point defects in U <sub>3</sub> Si <sub>2</sub> : effects on the mechanical and electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4287-4297.	1.3	7
71	Nanomechanical behavior of single crystalline SiC nanotubes revealed by molecular dynamics simulations. <i>Journal of Applied Physics</i> , 2008, 104, 093506.	1.1	6
72	First-principles study of He point-defects in HCP rare-earth metals. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011, 54, 827-830.	2.0	6

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73	Strong asymmetrical doping properties of spinel CoAl <sub>2</sub> O <sub>4</sub> . Journal of Applied Physics, 2012, 111, 093723.	1.1	6
74	Massive Scalar Quasinormal Modes of Higher Dimensional Small Dilatonic Black Hole. International Journal of Theoretical Physics, 2013, 52, 1370-1378.	0.5	6
75	First-principles study on the adsorption and dissociation of H <sub>2</sub> molecules on Be(0 0 0 1) surfaces. Computational Materials Science, 2016, 117, 251-258.	1.4	6
76	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> . Nanomaterials, 2019, 9, 196.	1.9	5
77	Effect of Copper Doping on Electronic Structure and Optical Absorption of Cd <sub>33</sub> Se <sub>33</sub> Quantum Dots. Nanomaterials, 2021, 11, 2531.	1.9	5
78	First-principles study on the strain-mediated g-C <sub>3</sub> N <sub>4</sub> /blue phosphorene heterostructures for promising photocatalytic performance. Journal of Physics Condensed Matter, 2021, 33, 485703.	0.7	5
79	Thermal Transport and Mechanical Properties of Layered Oxychalcogenides LaCuOX (X = S, Se, and Te). ACS Applied Energy Materials, 2022, 5, 6943-6951.	2.5	5
80	Effect of Thickness of Molybdenum Nano-Interlayer on Cohesion between Molybdenum/Titanium Multilayer Film and Silicon Substrate. Nanomaterials, 2019, 9, 616.	1.9	4
81	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. Nanomaterials, 2020, 10, 340.	1.9	4
82	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. Metals, 2021, 11, 553.	1.0	4
83	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.	1.1	3
84	Ion Technique for Identifying Gamma Detector Candidates. IEEE Transactions on Nuclear Science, 2009, 56, 920-925.	1.2	3
85	Interface engineering to enhance the oxygen evolution reaction under light irradiation. Applied Physics Letters, 2019, 115, 103901.	1.5	3
86	Probing the Origin of Gold Dissolution and Tunneling Across Ni <sub>2</sub> P Shell Using in situ Transmission Electron Microscopy. ACS Applied Materials & Interfaces, 2019, 11, 46947-46952.	4.0	2
87	An abnormal incorporation behavior of Th in Gd <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> : A first-principles study. Journal of the American Ceramic Society, 2020, 103, 1846-1853.	1.9	2
88	Defect formation and its effect on the thermodynamic properties of Pu <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> pyrochlore: a first-principles study. Journal of the American Ceramic Society, 2021, 104, 2301-2312.	1.9	2
89	Insight into the growth behaviors of MoS <sub>2</sub> nanograins influenced by step edges and atomic structure of the substrate. Nano Research, 2022, 15, 7646-7654.	5.8	2
90	Melamine foam loaded tellurium doped MoSe <sub>2</sub> as polysulphide reservoir interlayer for LiâˆS batteries. Materials Technology, 2022, 37, 2885-2892.	1.5	2

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91	A Comparative Study of Electron Radiation Responses of Pu <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> and La <sub>2</sub> Zr <sub>2</sub> O <sub>7</sub> : An abinitio Molecular Dynamics Study. <i>Materials</i> , 2021, 14, 1516.	1.3	1
92	In situsynchrotron X-ray diffraction analysis of deformation behaviour in Ti–Ni-based thin films. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 34-41.	1.0	0
93	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4751-4761.	1.5	0