

# Xiuwen Zhang

## List of Publications by Year in descending order

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83  
papers

4,501  
citations

126708

33  
h-index

106150

65  
g-index

84  
all docs

84  
docs citations

84  
times ranked

5797  
citing authors

#	ARTICLE	IF	CITATIONS
1	Stokes Shift in Inorganic Lead Halide Perovskites: Current Status and Perspective. ChemistryOpen, 2022, 11, e202100285.	0.9	11
2	Origin of the enhanced edge optical transition in transition metal dichalcogenide flakes. Journal of Materials Chemistry C, 2022, 10, 5303-5310.	2.7	1
3	Multiferroicity and giant in-plane negative Poisson's ratio in wurtzite monolayers. Npj Computational Materials, 2022, 8, .	3.5	7
4	Prediction of New Structures of the Na-Sb Alloy Anode for Na-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 11468-11474.	1.5	2
5	Highly Luminescent Zero-Dimensional Organic Copper Halide with Low-Loss Optical Waveguides and Highly Polarized Emission. , 2022, 4, 1446-1452.		21
6	Highly anisotropic gas sensing of atom-thin borophene: a first-principles study. Journal of Materials Chemistry C, 2021, 9, 1069-1076.	2.7	28
7	Two-dimensional topological insulators exfoliated from Na <sub>3</sub> Bi-like Dirac semimetals. Physical Chemistry Chemical Physics, 2021, 23, 10545-10550.	1.3	1
8	Design of memristor materials from ordered-vacancy zincblende semiconductors. Physical Review Materials, 2021, 5, .	0.9	4
9	Theoretical Study of Two-Dimensional ±-Tellurene with Pseudo-Heterospecies as a Promising Elemental Anchoring Material for Lithium-Sulfur Batteries. Journal of Physical Chemistry C, 2021, 125, 4623-4631.	1.5	12
10	Electrical Switch of Poisson's Ratio in IV-VI Monolayers via Pseudophase Transitions. Journal of Physical Chemistry Letters, 2021, 12, 3217-3223.	2.1	1
11	Dual Passivation Strategy for High Efficiency Inorganic CsPb <sub>2</sub> Br Solar Cells. Solar Rrl, 2021, 5, 2100112.	3.1	18
12	Efficient Dual-Band White-Light Emission with High Color Rendering from Zero-Dimensional Organic Copper Iodide. ACS Applied Materials & Interfaces, 2021, 13, 22749-22756.	4.0	57
13	Shape-Dependent Linear Dichroism Spectra of Colloidal Semiconductor Nanocrystals. Langmuir, 2021, 37, 7611-7616.	1.6	3
14	Crystalline chirality and interlocked double hourglass Weyl fermion in polyhedra-intercalated transition metal dichalcogenides. NPG Asia Materials, 2021, 13, .	3.8	12
15	Highly Luminescent Zero-Dimensional Organic Copper Halides for X-ray Scintillation. Journal of Physical Chemistry Letters, 2021, 12, 6919-6926.	2.1	95
16	Room-Temperature Ferroelectricity in 2D Metal-Tellurium-Oxyhalide Cd <sub>7</sub> Te <sub>7</sub> Cl <sub>8</sub> O <sub>17</sub> via Selenium-Induced Selective-Bonding Growth. ACS Nano, 2021, 15, 16525-16532.	7.3	12
17	Designing of 0D/2D mixed-dimensional van der waals heterojunction over ultrathin g-C <sub>3</sub> N <sub>4</sub> for high-performance flexible self-powered photodetector. Chemical Engineering Journal, 2021, 420, 129556.	6.6	34
18	Switchable electric polarization of phosphorene in mixed dimensional van der Waals heterostructure. Applied Surface Science, 2021, 563, 150276.	3.1	3

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19	MXene-based mixed-dimensional Schottky heterojunction towards self-powered flexible high-performance photodetector. <i>Materials Today Physics</i> , 2021, 21, 100479.	2.9	13
20	Theoretical Design of Inorganic Flexible Bulk Photovoltaic Materials. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10182-10189.	2.1	1
21	Realizing Near-Unity Quantum Efficiency of Zero-Dimensional Antimony Halides through Metal Halide Structural Modulation. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 58908-58915.	4.0	36
22	Recent advances in two-dimensional ferromagnetism: materials synthesis, physical properties and device applications. <i>Nanoscale</i> , 2020, 12, 2309-2327.	2.8	67
23	Designing Dirac semimetals with a honeycomb Na <sub>3</sub> Bi-lattice <i>via</i> isovalent cation substitution. <i>Journal of Materials Chemistry C</i> , 2020, 8, 1257-1264.	2.7	4
24	Dirac fermions in the antiferromagnetic spintronics material CuMnAs. <i>Physical Review B</i> , 2020, 102, .	1.1	8
25	Space-Confined Growth of 2D InI Showing High Sensitivity in Photodetection. <i>Advanced Electronic Materials</i> , 2020, 6, 2000284.	2.6	14
26	Design of Multifunctional Quinary Metal-Halide Perovskite Compounds Based on Cation-Anion Co-Ordering. <i>Chemistry of Materials</i> , 2020, 32, 5949-5957.	3.2	10
27	Photodetectors: Graphdiyne-Based Flexible Photodetectors with High Responsivity and Detectivity ( <i>Adv. Mater.</i> 23/2020). <i>Advanced Materials</i> , 2020, 32, 2070175.	11.1	5
28	The effects of interstitial iodine in hybrid perovskite hot carrier cooling: A non-adiabatic molecular dynamics study. <i>Journal of Chemical Physics</i> , 2020, 152, 091102.	1.2	15
29	Photophysics in Cs <sub>3</sub> Cu <sub>2</sub> X <sub>5</sub> (X = Cl, Br, or I): Highly Luminescent Self-Trapped Excitons from Local Structure Symmetrization. <i>Chemistry of Materials</i> , 2020, 32, 3462-3468.	3.2	177
30	Growth of Ultrathin Ternary Teallite (PbSnS <sub>2</sub> ) Flakes for Highly Anisotropic Optoelectronics. <i>Matter</i> , 2020, 2, 977-987.	5.0	53
31	Synthesis and optoelectronics of mixed-dimensional Bi/Te binary heterostructures. <i>Nanoscale Horizons</i> , 2020, 5, 847-856.	4.1	28
32	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. <i>Journal of Materials Chemistry C</i> , 2020, 8, 2798-2805.	2.7	16
33	Facet Control for Trap-State Suppression in Colloidal Quantum Dot Solids. <i>Advanced Functional Materials</i> , 2020, 30, 2000594.	7.8	60
34	Multifunctional VI-VI binary heterostructure-based self-powered pH-sensitive photo-detector. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5991-6000.	2.7	8
35	Graphdiyne-Based Flexible Photodetectors with High Responsivity and Detectivity. <i>Advanced Materials</i> , 2020, 32, e2001082.	11.1	171
36	Efficient and Reabsorption-Free Radioluminescence in Cs <sub>3</sub> Cu <sub>2</sub> I <sub>5</sub> Nanocrystals with Self-Trapped Excitons. <i>Advanced Science</i> , 2020, 7, 2000195.	5.6	282

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37	Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. <i>Physical Review B</i> , 2020, 102, .	1.1	4
38	Motif-Based Design of an Oxysulfide Class of Lithium Superionic Conductors: Toward Improved Stability and Record-High Li-Ion Conductivity. <i>Chemistry of Materials</i> , 2019, 31, 7265-7276.	3.2	25
39	Continuously Tuning Electronic Properties of Few-Layer Molybdenum Ditelluride with <i>in Situ</i> Aluminum Modification toward Ultrahigh Gain Complementary Inverters. <i>ACS Nano</i> , 2019, 13, 9464-9472.	7.3	36
40	Two-dimensional inorganic molecular crystals. <i>Nature Communications</i> , 2019, 10, 4728.	5.8	91
41	Epitaxial Growth of Topological Insulators on Semiconductors (Bi <sub>2</sub> Se <sub>3</sub> /Te@Se) toward High-Performance Photodetectors. <i>Small Methods</i> , 2019, 3, 1900349.	4.6	45
42	Detecting Semiconductor Nanoplatelets with Distinctive Crystal Structures and Thickness by Magnetic Circular Dichroism. <i>Journal of Physical Chemistry C</i> , 2019, 123, 29331-29336.	1.5	3
43	Self-Healable Black Phosphorus Photodetectors. <i>Advanced Functional Materials</i> , 2019, 29, 1906610.	7.8	48
44	Van der Waals Integration of Bismuth Quantum Dots-Decorated Tellurium Nanotubes (Te@Bi) Heterojunctions and Plasma-Enhanced Optoelectronic Applications. <i>Small</i> , 2019, 15, e1903233.	5.2	45
45	Growth of Highly Anisotropic 2D Ternary CaTe <sub>2</sub> O <sub>5</sub> Flakes on Molten Glass. <i>Advanced Functional Materials</i> , 2019, 29, 1903216.	7.8	13
46	Detecting electronic structure evolution of semiconductor nanocrystals by magnetic circular dichroism spectroscopy. <i>Nanoscale</i> , 2019, 11, 19380-19386.	2.8	6
47	Salt-Assisted Growth of Ultrathin GeSe Rectangular Flakes for Phototransistors with Ultrahigh Responsivity. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 23353-23360.	4.0	38
48	Enhanced Photodetection Properties of Tellurium@Selenium Roll-to-Roll Nanotube Heterojunctions. <i>Small</i> , 2019, 15, e1900902.	5.2	120
49	Lead-Free Perovskite Derivative Cs <sub>2</sub> SnCl <sub>6</sub> ·xBr <sub>x</sub> Single Crystals for Narrowband Photodetectors. <i>Advanced Optical Materials</i> , 2019, 7, 1900139.	3.6	123
50	Uncovering and tailoring hidden Rashba spin-orbit splitting in centrosymmetric crystals. <i>Nature Communications</i> , 2019, 10, 906.	5.8	53
51	Manipulation of Bi <sup>3+</sup> /In <sup>3+</sup> Transmutation and Mn <sup>2+</sup> -Doping Effect on the Structure and Optical Properties of Double Perovskite Cs <sub>2</sub> NaBi <sub>1-x</sub> ·xIn <sub>x</sub> Cl <sub>6</sub> . <i>Advanced Optical Materials</i> , 2019, 7, 1801435.	3.6	157
52	Design of p-type transparent conductors from inverted band structure: The case of inorganic metal halide perovskites. <i>Physical Review Materials</i> , 2019, 3, .	0.9	20
53	CsCu <sub>5</sub> Se <sub>3</sub> : A Copper-Rich Ternary Chalcogenide Semiconductor with Nearly Direct Band Gap for Photovoltaic Application. <i>Chemistry of Materials</i> , 2018, 30, 1121-1126.	3.2	30
54	Self-Limited Epitaxial Growth of Ultrathin Nonlayered CdS Flakes for High-Performance Photodetectors. <i>Advanced Functional Materials</i> , 2018, 28, 1800181.	7.8	86

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55	Theoretical design of multifunctional half-Heusler materials based on first-principles calculations. Chinese Physics B, 2018, 27, 127101.	0.7	5
56	Topological Insulators versus Topological Dirac Semimetals in Honeycomb Compounds. Journal of the American Chemical Society, 2018, 140, 13687-13694.	6.6	42
57	Distinct Excitonic Circular Dichroism between Wurtzite and Zinblend CdSe Nanoplatelets. Nano Letters, 2018, 18, 6665-6671.	4.5	68
58	Halide-Induced Self-Limited Growth of Ultrathin Nonlayered Ge Flakes for High-Performance Phototransistors. Journal of the American Chemical Society, 2018, 140, 12909-12914.	6.6	85
59	Approaches to design inorganic semiconductors while maintaining structural motifs. Journal of Semiconductors, 2018, 39, 071002.	2.0	1
60	Natural off-stoichiometry causes carrier doping in half-Heusler filled tetrahedral structures. Physical Review B, 2017, 95, .	1.1	61
61	Predicted electronic markers for polytypes of $\text{LaOBiS}_2$ examined via angle-resolved photoemission spectroscopy. Physical Review B, 2017, 95, .	1.1	18
62	The Enabling Electronic Motif for Topological Insulation in ABO <sub>3</sub> Perovskites. Advanced Functional Materials, 2017, 27, 1701266.	7.8	21
63	Excitonic Circular Dichroism of Chiral Quantum Rods. Journal of the American Chemical Society, 2017, 139, 8734-8739.	6.6	110
64	Transforming Common III-V and II-VI Semiconductor Compounds into Topological Heterostructures: The Case of CdTe/InSb Superlattices. Advanced Functional Materials, 2016, 26, 3259-3267.	7.8	27
65	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	1.2	29
66	Orbital mapping of energy bands and the truncated spin polarization in three-dimensional Rashba semiconductors. Physical Review B, 2016, 94, .	1.1	11
67	Minimal ingredients for orbital-texture switches at Dirac points in strong spin-orbit coupled materials. Npj Quantum Materials, 2016, 1, .	1.8	7
68	Polytypism in LaOBiS <sub>2</sub> -type compounds based on different three-dimensional stacking sequences of two-dimensional BiS <sub>2</sub> layers. Physical Review B, 2016, 93, .	1.1	34
69	Search and design of nonmagnetic centrosymmetric layered crystals with large local spin polarization. Physical Review B, 2015, 91, .	1.1	51
70	Emergence of a few distinct structures from a single formal structure type during high-throughput screening for stable compounds: The case of RbCuS and RbCuSe. Physical Review B, 2015, 92, .	1.1	10
71	Intrinsic Transparent Conductors without Doping. Physical Review Letters, 2015, 115, 176602.	2.9	36
72	Intrinsic Circular Polarization in Centrosymmetric Stacks of Transition-Metal Dichalcogenide Compounds. Physical Review Letters, 2015, 114, 087402.	2.9	53

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73	Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements. Nature Communications, 2015, 6, 7308.	5.8	89
74	Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. Nature Chemistry, 2015, 7, 308-316.	6.6	349
75	Prediction and Synthesis of Strain Tolerant RbCuTe Crystals Based on Rotation of One-Dimensional Nano Ribbons within a Three-Dimensional Inorganic Network. Journal of the American Chemical Society, 2015, 137, 11383-11390.	6.6	12
76	Hidden spin polarization in inversion-symmetric bulk crystals. Nature Physics, 2014, 10, 387-393.	6.5	400
77	Structurally unstable $\text{BiO}_3$ perovskites are predicted to be topological insulators but their stable structural forms are trivial band insulators.	1.1	21
78	Crystal structures and metastability of carbon-boron compounds $\text{C}_3\text{B}$ and $\text{C}_5\text{B}$ . Physical Review B, 2013, 87, .	1.1	22
79	Theoretical Prediction and Experimental Realization of New Stable Inorganic Materials Using the Inverse Design Approach. Journal of the American Chemical Society, 2013, 135, 10048-10054.	6.6	111
80	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. Physical Review B, 2012, 85, .	1.1	454
81	Sorting Stable versus Unstable Hypothetical Compounds: The Case of Multi-Functional ABX Half-Heusler Filled Tetrahedral Structures. Advanced Functional Materials, 2012, 22, 1425-1435.	7.8	107
82	Altered Reactivity and the Emergence of Ionic Metal Ordered Structures in Li-Cs at High Pressures. Physical Review Letters, 2010, 104, 245501.	2.9	17
83	Structure prediction and targeted synthesis: A new $\text{NaN}_2$ diazenide crystalline structure. Journal of Chemical Physics, 2010, 133, 194504.	1.2	17