

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
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84
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84
docs citations

84
times ranked

5797
citing authors

#	ARTICLE	IF	CITATIONS
1	Correcting density functional theory for accurate predictions of compound enthalpies of formation: Fitted elemental-phase reference energies. <i>Physical Review B</i> , 2012, 85, .	1.1	454
2	Hidden spin polarization in inversion-symmetric bulk crystals. <i>Nature Physics</i> , 2014, 10, 387-393.	6.5	400
3	Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds. <i>Nature Chemistry</i> , 2015, 7, 308-316.	6.6	349
4	Efficient and Reabsorption-Free Radioluminescence in Cs ₃ Cu ₂ I ₅ Nanocrystals with Self-Trapped Excitons. <i>Advanced Science</i> , 2020, 7, 2000195.	5.6	282
5	Photophysics in Cs ₃ Cu ₂ X ₅ (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
6	Graphdiyne-Based Flexible Photodetectors with High Responsivity and Detectivity. <i>Advanced Materials</i> , 2020, 32, e2001082.	11.1	171
7	Manipulation of Bi ³⁺ /In ³⁺ Transmutation and Mn ²⁺ Doping Effect on the Structure and Optical Properties of Double Perovskite Cs ₂ NaBi _{1-x} In _x Cl ₆ . <i>Advanced Optical Materials</i> , 2019, 7, 1801435.	3.6	157
8	Lead-Free Perovskite Derivative Cs ₂ SnCl ₆ ^x Br _x Single Crystals for Narrowband Photodetectors. <i>Advanced Optical Materials</i> , 2019, 7, 1900139.	3.6	123
9	Enhanced Photodetection Properties of Tellurium@Selenium Roll Nanotube Heterojunctions. <i>Small</i> , 2019, 15, e1900902.	5.2	120
10	Theoretical Prediction and Experimental Realization of New Stable Inorganic Materials Using the Inverse Design Approach. <i>Journal of the American Chemical Society</i> , 2013, 135, 10048-10054.	6.6	111
11	Excitonic Circular Dichroism of Chiral Quantum Rods. <i>Journal of the American Chemical Society</i> , 2017, 139, 8734-8739.	6.6	110
12	Sorting Stable versus Unstable Hypothetical Compounds: The Case of Multi-Functional ABX Half-Heusler Filled Tetrahedral Structures. <i>Advanced Functional Materials</i> , 2012, 22, 1425-1435.	7.8	107
13	Highly Luminescent Zero-Dimensional Organic Copper Halides for X-ray Scintillation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6919-6926.	2.1	95
14	Two-dimensional inorganic molecular crystals. <i>Nature Communications</i> , 2019, 10, 4728.	5.8	91
15	Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements. <i>Nature Communications</i> , 2015, 6, 7308.	5.8	89
16	Self-Limited Epitaxial Growth of Ultrathin Nonlayered CdS Flakes for High-Performance Photodetectors. <i>Advanced Functional Materials</i> , 2018, 28, 1800181.	7.8	86
17	Halide-Induced Self-Limited Growth of Ultrathin Nonlayered Ge Flakes for High-Performance Phototransistors. <i>Journal of the American Chemical Society</i> , 2018, 140, 12909-12914.	6.6	85
18	Distinct Excitonic Circular Dichroism between Wurtzite and Zinblend CdSe Nanoplatelets. <i>Nano Letters</i> , 2018, 18, 6665-6671.	4.5	68

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19	Recent advances in two-dimensional ferromagnetism: materials synthesis, physical properties and device applications. <i>Nanoscale</i> , 2020, 12, 2309-2327.	2.8	67
20	Natural off-stoichiometry causes carrier doping in half-Heusler filled tetrahedral structures. <i>Physical Review B</i> , 2017, 95, .	1.1	61
21	Facet Control for Trap- ϵ State Suppression in Colloidal Quantum Dot Solids. <i>Advanced Functional Materials</i> , 2020, 30, 2000594.	7.8	60
22	Efficient Dual-Band White-Light Emission with High Color Rendering from Zero-Dimensional Organic Copper Iodide. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 22749-22756.	4.0	57
23	Intrinsic Circular Polarization in Centrosymmetric Stacks of Transition-Metal Dichalcogenide Compounds. <i>Physical Review Letters</i> , 2015, 114, 087402.	2.9	53
24	Uncovering and tailoring hidden Rashba spin-orbit splitting in centrosymmetric crystals. <i>Nature Communications</i> , 2019, 10, 906.	5.8	53
25	Growth of Ultrathin Ternary Teallite (PbSnS ₂) Flakes for Highly Anisotropic Optoelectronics. <i>Matter</i> , 2020, 2, 977-987.	5.0	53
26	Search and design of nonmagnetic centrosymmetric layered crystals with large local spin polarization. <i>Physical Review B</i> , 2015, 91, .	1.1	51
27	Self-Healable Black Phosphorus Photodetectors. <i>Advanced Functional Materials</i> , 2019, 29, 1906610.	7.8	48
28	Epitaxial Growth of Topological Insulators on Semiconductors (Bi ₂ Se ₃ /Te@Se) toward High-Performance Photodetectors. <i>Small Methods</i> , 2019, 3, 1900349.	4.6	45
29	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
30	Topological Insulators versus Topological Dirac Semimetals in Honeycomb Compounds. <i>Journal of the American Chemical Society</i> , 2018, 140, 13687-13694.	6.6	42
31	Salt-Assisted Growth of Ultrathin GeSe Rectangular Flakes for Phototransistors with Ultrahigh Responsivity. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23353-23360.	4.0	38
32	Intrinsic Transparent Conductors without Doping. <i>Physical Review Letters</i> , 2015, 115, 176602.	2.9	36
33	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
34	Realizing Near-Unity Quantum Efficiency of Zero-Dimensional Antimony Halides through Metal Halide Structural Modulation. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 58908-58915.	4.0	36
35	Polytypism in LaOBiS ₂ -type compounds based on different three-dimensional stacking sequences of two-dimensional BiS ₂ layers. <i>Physical Review B</i> , 2016, 93, .	1.1	34
36	Designing of OD/2D mixed-dimensional van der waals heterojunction over ultrathin g-C ₃ N ₄ for high-performance flexible self-powered photodetector. <i>Chemical Engineering Journal</i> , 2021, 420, 129556.	6.6	34

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37	CsCu ₅ Se ₃ : A Copper-Rich Ternary Chalcogenide Semiconductor with Nearly Direct Band Gap for Photovoltaic Application. Chemistry of Materials, 2018, 30, 1121-1126.	3.2	30
38	Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures. Journal of Chemical Physics, 2016, 144, 144201.	1.2	29
39	Synthesis and optoelectronics of mixed-dimensional Bi/Te binary heterostructures. Nanoscale Horizons, 2020, 5, 847-856.	4.1	28
40	Highly anisotropic gas sensing of atom-thin borophene: a first-principles study. Journal of Materials Chemistry C, 2021, 9, 1069-1076.	2.7	28
41	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
42	Motif-Based Design of an Oxysulfide Class of Lithium Superionic Conductors: Toward Improved Stability and Record-High Li-Ion Conductivity. Chemistry of Materials, 2019, 31, 7265-7276.	3.2	25
43	Crystal structures and metastability of carbon-boron compounds C_3B and C_3B Structurally unstable C_3B https://doi.org/10.1103/PhysRevB.2013.07	1.1	22
44	BiO_3 perovskites are predicted to be topological insulators but their stable structural forms are trivial band insulators. Physical Review B, 2014, 90, .	1.1	21
45	The Enabling Electronic Motif for Topological Insulation in ABO ₃ Perovskites. Advanced Functional Materials, 2017, 27, 1701266.	7.8	21
46	Highly Luminescent Zero-Dimensional Organic Copper Halide with Low-Loss Optical Waveguides and Highly Polarized Emission. , 2022, 4, 1446-1452.		21
47	Design of p-type transparent conductors from inverted band structure: The case of inorganic metal halide perovskites. Physical Review Materials, 2019, 3, .	0.9	20
48	Predicted electronic markers for polytypes of $LaOBiS_2$ examined via angle-resolved photoemission spectroscopy. Physical Review B, 2017, 95, .	1.1	18
49	Dual Passivation Strategy for High Efficiency Inorganic CsPb ₂ Br Solar Cells. Solar Rrl, 2021, 5, 2100112.	3.1	18
50	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
51	Structure prediction and targeted synthesis: A new NanN ₂ diazenide crystalline structure. Journal of Chemical Physics, 2010, 133, 194504.	1.2	17
52	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. Journal of Materials Chemistry C, 2020, 8, 2798-2805.	2.7	16
53	The effects of interstitial iodine in hybrid perovskite hot carrier cooling: A non-adiabatic molecular dynamics study. Journal of Chemical Physics, 2020, 152, 091102.	1.2	15
54	Space-Confined Growth of 2D InI Showing High Sensitivity in Photodetection. Advanced Electronic Materials, 2020, 6, 2000284.	2.6	14

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55	Growth of Highly Anisotropic 2D Ternary CaTe ₂ O ₅ Flakes on Molten Glass. <i>Advanced Functional Materials</i> , 2019, 29, 1903216.	7.8	13
56	MXene-based mixed-dimensional Schottky heterojunction towards self-powered flexible high-performance photodetector. <i>Materials Today Physics</i> , 2021, 21, 100479.	2.9	13
57	Prediction and Synthesis of Strain Tolerant RbCuTe Crystals Based on Rotation of One-Dimensional Nano Ribbons within a Three-Dimensional Inorganic Network. <i>Journal of the American Chemical Society</i> , 2015, 137, 11383-11390.	6.6	12
58	Theoretical Study of Two-Dimensional $\hat{I}\pm$ -Tellurene with Pseudo-Heterospecies as a Promising Elemental Anchoring Material for Lithium-Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4623-4631.	1.5	12
59	Crystalline chirality and interlocked double hourglass Weyl fermion in polyhedra-intercalated transition metal dichalcogenides. <i>NPG Asia Materials</i> , 2021, 13, .	3.8	12
60	Room-Temperature Ferroelectricity in 2D Metal-Tellurium-Oxyhalide Cd ₇ Te ₇ Cl ₈ O ₁₇ via Selenium-Induced Selective-Bonding Growth. <i>ACS Nano</i> , 2021, 15, 16525-16532.	7.3	12
61	Orbital mapping of energy bands and the truncated spin polarization in three-dimensional Rashba semiconductors. <i>Physical Review B</i> , 2016, 94, .	1.1	11
62	Stokes Shift in Inorganic Lead Halide Perovskites: Current Status and Perspective. <i>ChemistryOpen</i> , 2022, 11, e202100285.	0.9	11
63	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. <i>Physical Review B</i> , 2015, 92, .	1.1	10
64	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
65	Dirac fermions in the antiferromagnetic spintronics material CuMnAs. <i>Physical Review B</i> , 2020, 102, .	1.1	8
66	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
67	Minimal ingredients for orbital-texture switches at Dirac points in strong spin-orbit coupled materials. <i>Npj Quantum Materials</i> , 2016, 1, .	1.8	7
68	Multiferroicity and giant in-plane negative Poisson's ratio in wurtzite monolayers. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	7
69	Detecting electronic structure evolution of semiconductor nanocrystals by magnetic circular dichroism spectroscopy. <i>Nanoscale</i> , 2019, 11, 19380-19386.	2.8	6
70	Theoretical design of multifunctional half-Heusler materials based on first-principles calculations. <i>Chinese Physics B</i> , 2018, 27, 127101.	0.7	5
71	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
72	Designing Dirac semimetals with a honeycomb Na ₃ Bi-lattice via isovalent cation substitution. <i>Journal of Materials Chemistry C</i> , 2020, 8, 1257-1264.	2.7	4

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73	Design of memristor materials from ordered-vacancy zincblende semiconductors. <i>Physical Review Materials</i> , 2021, 5, .	0.9	4
74	Ferri-chiral compounds with potentially switchable Dresselhaus spin splitting. <i>Physical Review B</i> , 2020, 102, .	1.1	4
75	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
76	Shape-Dependent Linear Dichroism Spectra of Colloidal Semiconductor Nanocrystals. <i>Langmuir</i> , 2021, 37, 7611-7616.	1.6	3
77	Switchable electric polarization of phosphorene in mixed dimensional van der Waals heterostructure. <i>Applied Surface Science</i> , 2021, 563, 150276.	3.1	3
78	Prediction of New Structures of the Na α -Sb Alloy Anode for Na-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2022, 126, 11468-11474.	1.5	2
79	Approaches to design inorganic semiconductors while maintaining structural motifs. <i>Journal of Semiconductors</i> , 2018, 39, 071002.	2.0	1
80	Two-dimensional topological insulators exfoliated from Na ₃ Bi-like Dirac semimetals. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10545-10550.	1.3	1
81	Electrical Switch of Poisson's Ratio in IV α -VI Monolayers via Pseudophase Transitions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3217-3223.	2.1	1
82	Theoretical Design of Inorganic Flexible Bulk Photovoltaic Materials. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10182-10189.	2.1	1
83	Origin of the enhanced edge optical transition in transition metal dichalcogenide flakes. <i>Journal of Materials Chemistry C</i> , 2022, 10, 5303-5310.	2.7	1