Naihua Miao

List of Publications by Year
in descending order

59 papers	2,461 citations	236925 25 h-index	206112 48 g-index
59 all docs	59 docs citations	59 times ranked	3190 citing authors

#	Article	IF	Citations
1	Computational design of twoâ€dimensional magnetic materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1545.	14.6	12
2	Breaking the linear scaling relations in MXene catalysts for efficient CO2 reduction. Chemical Engineering Journal, 2022, 429, 132171.	12.7	32
3	Computational design of double transition metal MXenes with intrinsic magnetic properties. Nanoscale Horizons, 2022, 7, 276-287.	8.0	29
4	Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation. Journal of the American Chemical Society, 2022, 144, 5878-5886.	13.7	21
5	ALKEMIE: An intelligent computational platform for accelerating materials discovery and design. Computational Materials Science, 2021, 186, 110064.	3.0	89
6	Pressure-mediated structural phase transitions and ultrawide indirectâ€“direct bandgaps in novel rare-earth oxyhalides. Journal of Materials Chemistry C, 2021, 9, 547-554.	5.5	9
7	Novel IVâ€“Vâ€“VI semiconductors with ultralow lattice thermal conductivity. Journal of Materials Chemistry C, 2021, 9, 4189-4199.	5.5	14
8	Novel metal oxides with promising high-temperature thermoelectric performance. Journal of Materials Chemistry C, 2021, 9, 12884-12894.	5.5	14
9	Engineering Carbon Materials for Electrochemical Oxygen Reduction Reactions. Advanced Energy Materials, 2021, 11, 2100695.	19.5	63
10	Functionalized Mo2B2 MBenes: Promising anchoring and electrocatalysis materials for Lithium-Sulfur battery. Applied Surface Science, 2021, 566, 150634.	6.1	29
11	Computational mining of Janus Sc₂C-based MXenes for spintronic, photocatalytic, and solar cell applications. Journal of Materials Chemistry A, 2021, 9, 10882-10892.	10.3	52
12	Quantifying the composition dependency of the ground-state structure, electronic property and phase-transition dynamics in ternary transition-metal-dichalcogenide monolayers. Journal of Materials Chemistry C, 2020, 8, 721-733.	5.5	7
13	Tunable phase transitions and high photovoltaic performance of two-dimensional In₂Ge₂Te₆ semiconductors. Nanoscale Horizons, 2020, 5, 1566-1573.	8.0	17
14	Stabilizing a Lithium Metal Battery by an In Situ Li₂S-modified Interfacial Layer via Amorphous-Sulfide Composite Solid Electrolyte. Nano Letters, 2020, 20, 8273-8281.	9.1	47
15	Composition-Gradient-Mediated Semiconductorâ€“Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers. ACS Applied Materials & Interfaces, 2020, 12, 45184-45191.	8.0	12
16	M2C-type MXenes: Promising catalysts for CO2 capture and reduction. Applied Surface Science, 2020, 521, 146436.	6.1	77
17	2D Magnetic Janus Semiconductors with Exotic Structural and Quantum-Phase Transitions. Journal of Physical Chemistry Letters, 2019, 10, 3922-3928.	4.6	28
18	Origin of high thermoelectric performance with a wide range of compositions for Bi_xSb_{2â^'x}Te₃ single quintuple layers. Physical Chemistry Chemical Physics, 2019, 21, 1315-1323.	2.8	7

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19	TlP₅: an unexplored direct band gap 2D semiconductor with ultra-high carrier mobility. Journal of Materials Chemistry C, 2019, 7, 639-644.	5.5	30
20	Local-ordering mediated configuration stability and elastic properties of aluminum-containing high entropy alloys. Intermetallics, 2019, 110, 106474.	3.9	6
21	The top-down synthesis of single-layered Cs₄CuSb₂Cl₁₂ halide perovskite nanocrystals for photoelectrochemical application. Nanoscale, 2019, 11, 5180-5187.	5.6	65
22	I-doped Cu2Se nanocrystals for high-performance thermoelectric applications. Journal of Alloys and Compounds, 2019, 772, 366-370.	5.5	47
23	Interaction of Trace Rareâ€Earth Dopants and Nanoheterogeneities Induces Giant Magnetostriction in Feâ€Ga Alloys. Advanced Functional Materials, 2018, 28, 1800858.	14.9	64
24	2D Intrinsic Ferromagnets from van der Waals Antiferromagnets. Journal of the American Chemical Society, 2018, 140, 2417-2420.	13.7	312
25	Insight into the role of W in amorphous GeTe for phase-change memory. Journal of Alloys and Compounds, 2018, 738, 270-276.	5.5	17
26	Structural stability and mechanical properties of Co3(Al, M) (Mâ€¯=â€¯Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W) compounds. Computational Materials Science, 2018, 148, 27-37.	3.0	24
27	Preparation and surface characteristics of Re3W matrix scandate cathode: An experimental and theoretical study. Applied Surface Science, 2018, 440, 763-769.	6.1	18
28	Strengthening mechanism of aluminum on elastic properties of NbVTiZr high-entropy alloys. Intermetallics, 2018, 92, 7-14.	3.9	44
29	High thermoelectric performance of few-quintuple Sb2Te3 nanofilms. Nano Energy, 2018, 43, 285-290.	16.0	51
30	Strengthening effects of alloying elements W and Re on Ni3Al: A first-principles study. Computational Materials Science, 2018, 144, 23-31.	3.0	27
31	Reduction, sintering and mechanical properties of rhenium-tungsten compounds. Journal of Alloys and Compounds, 2018, 735, 2685-2693.	5.5	24
32	Emission and evaporation properties of 75 at.% Re-25 at.% W mixed matrix impregnated cathode. Applied Surface Science, 2018, 427, 874-882.	6.1	20
33	Computational mining of the pressure effect on thermodynamic and thermoelectric properties of cubic Ca ₂ Si. Europhysics Letters, 2018, 123, 67003.	2.0	3
34	Coincident modulation of lattice and electron thermal transport performance in MXenes via surface functionalization. Physical Chemistry Chemical Physics, 2018, 20, 19689-19697.	2.8	18
35	Structural stability and thermoelectric property optimization of Ca₂Si. RSC Advances, 2017, 7, 8936-8943.	3.6	15
36	A photocatalyst of sulphur depleted monolayered molybdenum sulfide nanocrystals for dye degradation and hydrogen evolution reaction. Nano Energy, 2017, 38, 544-552.	16.0	90

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37	Insight into the role of oxygen in the phase-change material GeTe. Journal of Materials Chemistry C, 2017, 5, 3592-3599.	5.5	18
38	Strain-mediated type-I/type-II transition in MXene/Blue phosphorene van der Waals heterostructures for flexible optical/electronic devices. Journal of Materials Chemistry C, 2017, 5, 978-984.	5.5	155
39	Few-layer arsenic trichalcogenides: Emerging two-dimensional semiconductors with tunable indirect-direct band-gaps. Journal of Alloys and Compounds, 2017, 699, 554-560.	5.5	33
40	An experimental and first-principles investigation of noncentrosymmetric cubic Re3W. Journal of Alloys and Compounds, 2017, 728, 984-991.	5.5	3
41	Tunable Magnetism and Extraordinary Sunlight Absorbance in Indium Triphosphide Monolayer. Journal of the American Chemical Society, 2017, 139, 11125-11131.	13.7	265
42	Pressure-Induced Destabilization and Anomalous Lattice Distortion in TcO2. Inorganic Chemistry, 2017, 56, 9973-9978.	4.0	1
43	Reduction of thermal conductivity in YxSb2â€“xTe3 for phase change memory. Journal of Applied Physics, 2017, 122, .	2.5	21
44	Adsorption and diffusion of hydrogen and oxygen in FCC-Co: a first-principles study. Physical Chemistry Chemical Physics, 2017, 19, 32404-32411.	2.8	11
45	Pressure-induced semimetal-semiconductor transition and enhancement of thermoelectric performance in Î±-MgAgSb. Applied Physics Letters, 2016, 108, .	3.3	19
46	First-Principles Study of the Thermoelectric Properties of SrRuO3. Journal of Physical Chemistry C, 2016, 120, 9112-9121.	3.1	27
47	Sulfur-Depleted Monolayered Molybdenum Disulfide Nanocrystals for Superelectrochemical Hydrogen Evolution Reaction. ACS Nano, 2016, 10, 8929-8937.	14.6	140
48	The pressure induced twisted distortion in the flexible oxide Tc2O7. CrystEngComm, 2016, 18, 328-333.	2.6	5
49	Optimization of Thermoelectric Properties of MgAgSb-Based Materials: A First-Principles Investigation. Journal of Physical Chemistry C, 2015, 119, 14017-14022.	3.1	12
50	Polyhedral transformation and phase transition in TcO₂. RSC Advances, 2015, 5, 1690-1696.	3.6	9
51	First-principles study of the lattice dynamical properties of strontium ruthenate. Journal of Physics Condensed Matter, 2014, 26, 035401.	1.8	29
52	Electronic, elastic, thermodynamic properties and structure disorder of Î³-AlON solid solution from ab initio calculations. Journal of Alloys and Compounds, 2013, 548, 228-234.	5.5	14
53	Thermodynamic evaluation and optimization of the (Na+X) binary systems (X=Ag, Ca, In, Sn, Zn) using combined Calphad and first-principles methods of calculation. Journal of Chemical Thermodynamics, 2013, 66, 22-33.	2.0	23
54	Theoretical investigation on the transition-metal borides with Ta3B4-type structure: A class of hard and refractory materials. Computational Materials Science, 2011, 50, 1559-1566.	3.0	169

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55	Mechanical properties and electronic structure of the incompressible rhenium carbides and nitrides: A first-principles study. Solid State Communications, 2011, 151, 1842-1845.	1.9	20
56	Investigation on Ge5â^'x Sb x Te5 phase-change materials byÂfirst-principles method. Applied Physics A: Materials Science and Processing, 2010, 99, 961-964.	2.3	4
57	Phase stability and electronic structure of Si2Sb2Te5 phase-change material. Journal of Physics and Chemistry of Solids, 2010, 71, 1165-1167.	4.0	2
58	First-principles investigation on the phase stability and chemical bonding of phase-change random alloys. Solid State Communications, 2010, 150, 1375-1377.	1.9	10
59	Ab initio study of the structure and chemical bonding of stable Ge3Sb2Te6. Physical Chemistry Chemical Physics, 2010, 12, 1585.	2.8	37