

Naihua Miao

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4973362/publications.pdf>

Version: 2024-02-01

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	2D Intrinsic Ferromagnets from van der Waals Antiferromagnets. <i>Journal of the American Chemical Society</i> , 2018, 140, 2417-2420.	13.7	312
2	Tunable Magnetism and Extraordinary Sunlight Absorbance in Indium Triphosphide Monolayer. <i>Journal of the American Chemical Society</i> , 2017, 139, 11125-11131.	13.7	265
3	Theoretical investigation on the transition-metal borides with Ta ₃ B ₄ -type structure: A class of hard and refractory materials. <i>Computational Materials Science</i> , 2011, 50, 1559-1566.	3.0	169
4	Strain-mediated type-I/type-II transition in MXene/Blue phosphorene van der Waals heterostructures for flexible optical/electronic devices. <i>Journal of Materials Chemistry C</i> , 2017, 5, 978-984.	5.5	155
5	Sulfur-Depleted Monolayered Molybdenum Disulfide Nanocrystals for Superelectrochemical Hydrogen Evolution Reaction. <i>ACS Nano</i> , 2016, 10, 8929-8937.	14.6	140
6	A photocatalyst of sulphur depleted monolayered molybdenum sulfide nanocrystals for dye degradation and hydrogen evolution reaction. <i>Nano Energy</i> , 2017, 38, 544-552.	16.0	90
7	ALKEMIE: An intelligent computational platform for accelerating materials discovery and design. <i>Computational Materials Science</i> , 2021, 186, 110064.	3.0	89
8	M ₂ C-type MXenes: Promising catalysts for CO ₂ capture and reduction. <i>Applied Surface Science</i> , 2020, 521, 146436.	6.1	77
9	The top-down synthesis of single-layered Cs ₄ CuSb ₂ Cl ₁₂ halide perovskite nanocrystals for photoelectrochemical application. <i>Nanoscale</i> , 2019, 11, 5180-5187.	5.6	65
10	Interaction of Trace Rare-Earth Dopants and Nanoheterogeneities Induces Giant Magnetostriction in Fe-Ga Alloys. <i>Advanced Functional Materials</i> , 2018, 28, 1800858.	14.9	64
11	Engineering Carbon Materials for Electrochemical Oxygen Reduction Reactions. <i>Advanced Energy Materials</i> , 2021, 11, 2100695.	19.5	63
12	Computational mining of Janus Sc ₂ C-based MXenes for spintronic, photocatalytic, and solar cell applications. <i>Journal of Materials Chemistry A</i> , 2021, 9, 10882-10892.	10.3	52
13	High thermoelectric performance of few-quintuple Sb ₂ Te ₃ nanofilms. <i>Nano Energy</i> , 2018, 43, 285-290.	16.0	51
14	I-doped Cu ₂ Se nanocrystals for high-performance thermoelectric applications. <i>Journal of Alloys and Compounds</i> , 2019, 772, 366-370.	5.5	47
15	Stabilizing a Lithium Metal Battery by an In Situ Li ₂ S-modified Interfacial Layer via Amorphous-Sulfide Composite Solid Electrolyte. <i>Nano Letters</i> , 2020, 20, 8273-8281.	9.1	47
16	Strengthening mechanism of aluminum on elastic properties of NbVTiZr high-entropy alloys. <i>Intermetallics</i> , 2018, 92, 7-14.	3.9	44
17	Ab initio study of the structure and chemical bonding of stable Ge ₃ Sb ₂ Te ₆ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1585.	2.8	37
18	Few-layer arsenic trichalcogenides: Emerging two-dimensional semiconductors with tunable indirect-direct band-gaps. <i>Journal of Alloys and Compounds</i> , 2017, 699, 554-560.	5.5	33

#	ARTICLE	IF	CITATIONS
19	Breaking the linear scaling relations in MXene catalysts for efficient CO ₂ reduction. <i>Chemical Engineering Journal</i> , 2022, 429, 132171.	12.7	32
20	TiP ₅ : an unexplored direct band gap 2D semiconductor with ultra-high carrier mobility. <i>Journal of Materials Chemistry C</i> , 2019, 7, 639-644.	5.5	30
21	First-principles study of the lattice dynamical properties of strontium ruthenate. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 035401.	1.8	29
22	Functionalized Mo ₂ B ₂ MBenes: Promising anchoring and electrocatalysis materials for Lithium-Sulfur battery. <i>Applied Surface Science</i> , 2021, 566, 150634.	6.1	29
23	Computational design of double transition metal MXenes with intrinsic magnetic properties. <i>Nanoscale Horizons</i> , 2022, 7, 276-287.	8.0	29
24	2D Magnetic Janus Semiconductors with Exotic Structural and Quantum-Phase Transitions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3922-3928.	4.6	28
25	First-Principles Study of the Thermoelectric Properties of SrRuO ₃ . <i>Journal of Physical Chemistry C</i> , 2016, 120, 9112-9121.	3.1	27
26	Strengthening effects of alloying elements W and Re on Ni ₃ Al: A first-principles study. <i>Computational Materials Science</i> , 2018, 144, 23-31.	3.0	27
27	Structural stability and mechanical properties of Co ₃ (Al, M) (M = Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W) compounds. <i>Computational Materials Science</i> , 2018, 148, 27-37.	3.0	24
28	Reduction, sintering and mechanical properties of rhenium-tungsten compounds. <i>Journal of Alloys and Compounds</i> , 2018, 735, 2685-2693.	5.5	24
29	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. <i>Journal of Chemical Thermodynamics</i> , 2013, 66, 22-33.	2.0	23
30	Reduction of thermal conductivity in Y _{1-x} Sb _{2x} Te ₃ for phase change memory. <i>Journal of Applied Physics</i> , 2017, 122, .	2.5	21
31	Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation. <i>Journal of the American Chemical Society</i> , 2022, 144, 5878-5886.	13.7	21
32	Mechanical properties and electronic structure of the incompressible rhenium carbides and nitrides: A first-principles study. <i>Solid State Communications</i> , 2011, 151, 1842-1845.	1.9	20
33	Emission and evaporation properties of 75 at.% Re-25 at.% W mixed matrix impregnated cathode. <i>Applied Surface Science</i> , 2018, 427, 874-882.	6.1	20
34	Pressure-induced semimetal-semiconductor transition and enhancement of thermoelectric performance in MgAgSb . <i>Applied Physics Letters</i> , 2016, 108, .	3.3	19
35	Insight into the role of oxygen in the phase-change material GeTe. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3592-3599.	5.5	18
36	Preparation and surface characteristics of Re ₃ W matrix scandate cathode: An experimental and theoretical study. <i>Applied Surface Science</i> , 2018, 440, 763-769.	6.1	18

#	ARTICLE	IF	CITATIONS
37	Coincident modulation of lattice and electron thermal transport performance in MXenes <i>via</i> surface functionalization. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 19689-19697.	2.8	18
38	Insight into the role of W in amorphous GeTe for phase-change memory. <i>Journal of Alloys and Compounds</i> , 2018, 738, 270-276.	5.5	17
39	Tunable phase transitions and high photovoltaic performance of two-dimensional $\text{In}_2\text{Ge}_2\text{Te}_6$ semiconductors. <i>Nanoscale Horizons</i> , 2020, 5, 1566-1573.	8.0	17
40	Structural stability and thermoelectric property optimization of Ca_2Si . <i>RSC Advances</i> , 2017, 7, 8936-8943.	3.6	15
41	Electronic, elastic, thermodynamic properties and structure disorder of $\hat{\Gamma}^3$ -AlON solid solution from ab initio calculations. <i>Journal of Alloys and Compounds</i> , 2013, 548, 228-234.	5.5	14
42	Novel IV-VI semiconductors with ultralow lattice thermal conductivity. <i>Journal of Materials Chemistry C</i> , 2021, 9, 4189-4199.	5.5	14
43	Novel metal oxides with promising high-temperature thermoelectric performance. <i>Journal of Materials Chemistry C</i> , 2021, 9, 12884-12894.	5.5	14
44	Optimization of Thermoelectric Properties of MgAgSb-Based Materials: A First-Principles Investigation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 14017-14022.	3.1	12
45	Composition-Gradient-Mediated Semiconductor-Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 45184-45191.	8.0	12
46	Computational design of two-dimensional magnetic materials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2022, 12, e1545.	14.6	12
47	Adsorption and diffusion of hydrogen and oxygen in FCC-Co: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32404-32411.	2.8	11
48	First-principles investigation on the phase stability and chemical bonding of phase-change random alloys. <i>Solid State Communications</i> , 2010, 150, 1375-1377.	1.9	10
49	Polyhedral transformation and phase transition in TcO_2 . <i>RSC Advances</i> , 2015, 5, 1690-1696.	3.6	9
50	Pressure-mediated structural phase transitions and ultrawide indirect-direct bandgaps in novel rare-earth oxyhalides. <i>Journal of Materials Chemistry C</i> , 2021, 9, 547-554.	5.5	9
51	Origin of high thermoelectric performance with a wide range of compositions for $\text{Bi}_x\text{Sb}_{2-x}\text{Te}_3$ single quintuple layers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1315-1323.	2.8	7
52	Quantifying the composition dependency of the ground-state structure, electronic property and phase-transition dynamics in ternary transition-metal-dichalcogenide monolayers. <i>Journal of Materials Chemistry C</i> , 2020, 8, 721-733.	5.5	7
53	Local-ordering mediated configuration stability and elastic properties of aluminum-containing high entropy alloys. <i>Intermetallics</i> , 2019, 110, 106474.	3.9	6
54	The pressure induced twisted distortion in the flexible oxide Tc_2O_7 . <i>CrystEngComm</i> , 2016, 18, 328-333.	2.6	5

#	ARTICLE	IF	CITATIONS
55	Investigation on Ge _{5-x} Sb _x Te ₅ phase-change materials by first-principles method. Applied Physics A: Materials Science and Processing, 2010, 99, 961-964.	2.3	4
56	An experimental and first-principles investigation of noncentrosymmetric cubic Re ₃ W. Journal of Alloys and Compounds, 2017, 728, 984-991.	5.5	3
57	Computational mining of the pressure effect on thermodynamic and thermoelectric properties of cubic Ca ₂ Si. Europhysics Letters, 2018, 123, 67003.	2.0	3
58	Phase stability and electronic structure of Si ₂ Sb ₂ Te ₅ phase-change material. Journal of Physics and Chemistry of Solids, 2010, 71, 1165-1167.	4.0	2
59	Pressure-Induced Destabilization and Anomalous Lattice Distortion in TcO ₂ . Inorganic Chemistry, 2017, 56, 9973-9978.	4.0	1