Yu Xie

List of Publications by Year
in descending order

66 papers	11,120 citations	81743 39 h-index	102304 66 g-index
67 all docs	67 docs citations	67 times ranked	11747 citing authors

#	Article	IF	Citations
1	Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes). ACS Nano, 2015, 9, 9507-9516.	7.3	1,395
2	A library of atomically thin metal chalcogenides. Nature, 2018, 556, 355-359.	13.7	1,225
3	Role of Surface Structure on Li-Ion Energy Storage Capacity of Two-Dimensional Transition-Metal Carbides. Journal of the American Chemical Society, 2014, 136, 6385-6394.	6.6	1,164
4	Prediction and Characterization of MXene Nanosheet Anodes for Non-Lithium-Ion Batteries. ACS Nano, 2014, 8, 9606-9615.	7.3	814
5	Atomic Defects in Monolayer Titanium Carbide (Ti₃C₂T_x) MXene. ACS Nano, 2016, 10, 9193-9200.	7.3	785
6	Transparent dense sodium. Nature, 2009, 458, 182-185.	13.7	710
7	Hybrid density functional study of structural and electronic properties of functionalized Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow		

#	Article	IF	Citations
19	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. Nature Communications, 2018, 9, 2266.	5.8	125
20	Nanoscale Elastic Changes in 2D Ti₃C₂T_x (MXene) Pseudocapacitive Electrodes. Advanced Energy Materials, 2016, 6, 1502290.	10.2	117
21	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
22	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. Physical Review B, 2005, 72, .	1.1	96
23	Advances and challenges in 2D MXenes: From structures to energy storage and conversions. Nano Today, 2021, 40, 101273.	6.2	91
24	Global minimization of gold clusters by combining neural network potentials and the basin-hopping method. Nanoscale, 2015, 7, 14817-14821.	2.8	90
25	Rational defect and anion chemistries in Co3O4 for enhanced oxygen evolution reaction. Applied Catalysis B: Environmental, 2021, 281, 119535.	10.8	90
26	Double transition metal MXenes with wide band gaps and novel magnetic properties. Nanoscale, 2018, 10, 11962-11968.	2.8	88
27	Density functional study of elastic and vibrational properties of the Heusler-type alloys<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub>	1.1	77
28	Computational discovery of a dynamically stable cubic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SH</mml:mi><mml:mn>3</mml:mn></mml:msub></mml: -like high-temperature superconductor at 100ÂGPa via <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml intercalation. Physical Review B, 2020, 101, .	1.1	73
29	A Promising Carbon/gâ€C₃N₄ Composite Negative Electrode for a Longâ€Life Sodiumâ€Ion Battery. Angewandte Chemie - International Edition, 2019, 58, 13727-13733.	7.2	70
30	Novel High Pressure Structures and Superconductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ca</mml:mi><mml:msub><mml:mi>Li</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2010, 104, 177005.	2.9	64
31	Exotic high pressure behavior of light alkali metals, lithium and sodium. European Physical Journal B, 2011, 81, 1-14.	0.6	62
32	Superconductivity of lithium-doped hydrogen under high pressure. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 104-111.	0.2	59
33	Edge Segregated Polymorphism in 2D Molybdenum Carbide. Advanced Materials, 2019, 31, e1808343.	11.1	56
34	Ab Initio Quality NMR Parameters in Solid-State Materials Using a High-Dimensional Neural-Network Representation. Journal of Chemical Theory and Computation, 2016, 12, 765-773.	2.3	51
35	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
36	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. Journal of Physical Chemistry Letters, 2020, 11, 8710-8720.	2.1	45

#	Article	IF	Citations
37	First-principles study of the lattice dynamics, thermodynamic properties and electron-phonon coupling of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	42
38	Electronic structures, lattice dynamics, and electronâ€“phonon coupling of simple cubic Ca under pressure. Solid State Communications, 2008, 146, 181-185.	0.9	41
39	A General Route to Prepare Lowâ€Rutheniumâ€Content Bimetallic Electrocatalysts for pHâ€Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. Angewandte Chemie, 2020, 132, 1735-1743.	1.6	40
40	Chemically Tuning Stability and Superconductivity of Pâ€“H Compounds. Journal of Physical Chemistry Letters, 2020, 11, 935-939.	2.1	40
41	Rational understanding of the catalytic mechanism of molybdenum carbide in polysulfide conversion in lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2020, 8, 11818-11823.	5.2	38
42	Electronic and crystal structures of osmium under high pressure. Physical Review B, 2005, 72, .	1.1	35
43	Machine learning electron density in sulfur crosslinked carbon nanotubes. Composites Science and Technology, 2018, 166, 3-9.	3.8	35
44	Pressure-induced high-temperature superconductivity retained without pressure in FeSe single crystals. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	30
45	Salt-Assisted MoS₂ Growth: Molecular Mechanisms from the First Principles. Journal of the American Chemical Society, 2022, 144, 7497-7503.	6.6	30
46	A Promising Carbon/gâ€C₃N₄ Composite Negative Electrode for a Longâ€Life Sodiumâ€Ion Battery. Angewandte Chemie, 2019, 131, 13865-13871.	1.6	29
47	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied usingab initiocalculations. Physical Review B, 2007, 75, .	1.1	28
48	Origin of bcc to fcc phase transition under pressure in alkali metals. New Journal of Physics, 2008, 10, 063022.	1.2	26
49	Pressure-induced enhancement of electron-phonon coupling in superconductingCaC6from first principles. Physical Review B, 2006, 74, .	1.1	25
50	Na5YSi4O12: A sodium superionic conductor for ultrastable quasi-solid-state sodium-ion batteries. Energy Storage Materials, 2021, 41, 196-202.	9.5	23
51	Graphene as an electrochemical transfer layer. Carbon, 2019, 141, 266-273.	5.4	17
52	The effects of pressure on the electronic, transport and dynamical properties of AuX₂(X =) Tj ETQq0 0 0 rgBT /Overlock 10	0.7	15
53	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	1.1	15
54	Aqueous nickel-ion battery with Na2V6O16Â·2H2O nanowire as high-capacity and zero-strain host material. Chemical Engineering Journal, 2021, 413, 127441.	6.6	13

#	Article	IF	Citations
55	Superconductivity and lattice instability in face-centered cubic lanthanum under high pressure. Journal of Physics Condensed Matter, 2007, 19, 425234.	0.7	12
56	Prediction of superconductivity in pressure-induced new silicon boride phases. Physical Review B, 2020, 101, .	1.1	12
57	Particle Swarm Predictions of a SrB₈ Monolayer with 12-Fold Metal Coordination. Journal of the American Chemical Society, 2022, 144, 11120-11128.	6.6	12
58	Competition among Refined Hollow Structures in Schiff Base Polymer Derived Carbon Microspheres. Nano Letters, 2022, 22, 3691-3698.	4.5	11
59	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. Physical Review B, 2019, 99, .	1.1	10
60	First-principles study of high-pressure phase stability and superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>4</mml:mn></mml:n mathvariant="normal">I</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, .	1.1	9
61	Gas-Phase â€œPrehistoryâ€•and Molecular Precursors in Monolayer Metal Dichalcogenides Synthesis: The Case of MoS₂. ACS Nano, 2021, 15, 10525-10531.	7.3	9
62	Pressure-induced decomposition of binary lanthanum intermetallic compounds. Physical Review B, 2020, 101, .	1.1	9
63	Atomic Defects and Edge Structure in Single-layer Ti₃C₂T_x MXene. Microscopy and Microanalysis, 2017, 23, 1704-1705.	0.2	7
64	Ab initio high-throughput screening of transition metal double chalcogenide monolayers as highly efficient bifunctional catalysts for photochemical and photoelectrochemical water splitting. Journal of Materials Chemistry A, 2022, 10, 14060-14069.	5.2	7
65	Crystal structures and superconductivity of carbonaceous sulfur hydrides at pressures up to 300 GPa. Physical Review B, 2022, 105, .	1.1	3
66	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	1.1	2