Yu Xie

List of Publications by Year
in descending order

66	11,120	81839	102432
papers	citations	39 h-index	66 g-index

67	67	67	11747
all docs	docs citations	times ranked	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		

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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

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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

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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