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	Crystal structures and superconductivity of carbonaceous sulfur hydrides at pressures up to 300 GPa. Physical Review B, 2022, 105, .	1.1	3
2	High-Temperature Superconducting Phase in Clathrate Calcium Hydride <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CaH</mml:mi></mml:mrow><mml:mrow><mml:mn>6</mml:mn></m up to 215ÂK at a Pressure of 172ÂGPa. Physical Review Letters, 2022, 128, 167001.	2.9	149
3	Salt-Assisted MoS₂ Growth: Molecular Mechanisms from the First Principles. Journal of the American Chemical Society, 2022, 144, 7497-7503.	6.6	30
4	Competition among Refined Hollow Structures in Schiff Base Polymer Derived Carbon Microspheres. Nano Letters, 2022, 22, 3691-3698.	4.5	11
5	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
6	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
7	Rational defect and anion chemistries in Co3O4 for enhanced oxygen evolution reaction. Applied Catalysis B: Environmental, 2021, 281, 119535.	10.8	90
8	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
9	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	1.1	15
10	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
11	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	1.1	2
12	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
13	Na5YSi4O12: A sodium superionic conductor for ultrastable quasi-solid-state sodium-ion batteries. Energy Storage Materials, 2021, 41, 196-202.	9.5	23
14	Advances and challenges in 2D MXenes: From structures to energy storage and conversions. Nano Today, 2021, 40, 101273.	6.2	91
15	A General Route to Prepare Lowâ€Ruthâ€Content Bimetallic Electrocatalysts for pHâ€Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. Angewandte Chemie, 2020, 132, 1735-1743.	1.6	40
16	A General Route to Prepare Lowâ€Ruthâ€Content Bimetallic Electrocatalysts for pHâ€Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. Angewandte Chemie - International Edition, 2020, 59, 1718-1726.	7.2	452
17	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
18	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

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19	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
20	Chemically Tuning Stability and Superconductivity of Pâ€“H Compounds. Journal of Physical Chemistry Letters, 2020, 11, 935-939.	2.1	40
21	Prediction of superconductivity in pressure-induced new silicon boride phases. Physical Review B, 2020, 101, .	1.1	12
22	Pressure-induced decomposition of binary lanthanum intermetallic compounds. Physical Review B, 2020, 101, .	1.1	9
23	A Promising Carbon/gâ€C₃N₄ Composite Negative Electrode for a Longâ€Life Sodiumâ€Ion Battery. Angewandte Chemie, 2019, 131, 13865-13871.	1.6	29
24	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
25	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. Physical Review Letters, 2019, 123, 097001.	2.9	255
26	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. Physical Review B, 2019, 99, .	1.1	10
27	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
28	Edge Segregated Polymorphism in 2D Molybdenum Carbide. Advanced Materials, 2019, 31, e1808343.	11.1	56
29	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:msub><mml:mathvariant="normal">I</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, .	1.1	9
30	Graphene as an electrochemical transfer layer. Carbon, 2019, 141, 266-273.	5.4	17
31	A library of atomically thin metal chalcogenides. Nature, 2018, 556, 355-359.	13.7	1,225
32	Machine learning electron density in sulfur crosslinked carbon nanotubes. Composites Science and Technology, 2018, 166, 3-9.	3.8	35
33	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. Nature Communications, 2018, 9, 2266.	5.8	125
34	Double transition metal MXenes with wide band gaps and novel magnetic properties. Nanoscale, 2018, 10, 11962-11968.	2.8	88
35	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
36	Multimodality of Structural, Electrical, and Gravimetric Responses of Intercalated MXenes to Water. ACS Nano, 2017, 11, 11118-11126.	7.3	183

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37	Atomic Defects and Edge Structure in Single-layer Ti₃C₂T_x MXene. Microscopy and Microanalysis, 2017, 23, 1704-1705.	0.2	7
38	Atomic Defects in Monolayer Titanium Carbide (Ti₃C₂T_x) MXene. ACS Nano, 2016, 10, 9193-9200.	7.3	785
39	Nanoscale Elastic Changes in 2D Ti₃C₂T_x (MXene) Pseudocapacitive Electrodes. Advanced Energy Materials, 2016, 6, 1502290.	10.2	117
40	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
41	Effect of Metal Ion Intercalation on the Structure of MXene and Water Dynamics on its Internal Surfaces. ACS Applied Materials & Interfaces, 2016, 8, 8859-8863.	4.0	225
42	Control of electronic properties of 2D carbides (MXenes) by manipulating their transition metal layers. Nanoscale Horizons, 2016, 1, 227-234.	4.1	394
43	Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes). ACS Nano, 2015, 9, 9507-9516.	7.3	1,395
44	Computational discovery of ferromagnetic semiconducting single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrSnTe</mml:mi><mml:mn>3</mml:mn></mml:msub></ Physical Review B, 2015, 92, .	3.1	212
45	Global minimization of gold clusters by combining neural network potentials and the basin-hopping method. Nanoscale, 2015, 7, 14817-14821.	2.8	90
46	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
47	Prediction and Characterization of MXene Nanosheet Anodes for Non-Lithium-Ion Batteries. ACS Nano, 2014, 8, 9606-9615.	7.3	814
48	Superconductivity of lithium-doped hydrogen under high pressure. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 104-111.	0.2	59
49	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
50	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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55	Transparent dense sodium. Nature, 2009, 458, 182-185.	13.7	710
56	Novel High Pressure Structures of Polymeric Nitrogen. Physical Review Letters, 2009, 102, 065501.	2.9	226
57	Electronic structures, lattice dynamics, and electronâ€“phonon coupling of simple cubic Ca under pressure. Solid State Communications, 2008, 146, 181-185.	0.9	41
58	Origin of bcc to fcc phase transition under pressure in alkali metals. New Journal of Physics, 2008, 10, 063022.	1.2	26
59	High-pressure structures of lithium, potassium, and rubidium predicted by anab initioevolutionary algorithm. Physical Review B, 2008, 78, .	1.1	132
60	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied usingab initiocalculations. Physical Review B, 2007, 75, .	1.1	28
61	Superconductivity and lattice instability in face-centered cubic lanthanum under high pressure. Journal of Physics Condensed Matter, 2007, 19, 425234.	0.7	12
62	The effects of pressure on the electronic, transport and dynamical properties of AuX₂(X =) Tj ETQq0 0 0 rgBT /Overlock 10	0.7	15
63	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
64	Pressure-induced enhancement of electron-phonon coupling in superconductingCaC6from first principles. Physical Review B, 2006, 74, .	1.1	25
65	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
66	Electronic and crystal structures of osmium under high pressure. Physical Review B, 2005, 72, .	1.1	35