Xiang-Feng Zhou

List of Publications by Year
in descending order

66 papers	5,803 citations	172207 29 h-index	102304 66 g-index
68 all docs	68 docs citations	68 times ranked	6020 citing authors

#	Article	IF	Citations
1	Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. Science, 2015, 350, 1513-1516.	6.0	2,047
2	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. Physical Review Letters, 2014, 112, .	2.9	497
3	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5â€“6â€“7 Carbon Rings with Distorted Dirac Cones. Nano Letters, 2015, 15, 6182-6186.	4.5	482
4	A stable compound of helium and sodium at high pressure. Nature Chemistry, 2017, 9, 440-445.	6.6	276
5	Novel Superhard Carbon: C-Centered Orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>8</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2011, 107, 215502.	2.9	225
6	Strain effects on borophene: ideal strength, negative Possionâ€™s ratio and phonon instability. New Journal of Physics, 2016, 18, 073016.	1.2	174
7	Hierarchically structured diamond composite with exceptional toughness. Nature, 2020, 582, 370-374.	13.7	141
8	Ab initiostudy of the formation of transparent carbon under pressure. Physical Review B, 2010, 82, .	1.1	119
9	First-principles study of electronic structure and optical properties of heterodiamondBC2N. Physical Review B, 2006, 73, .	1.1	113
10	Three Dimensional Carbon-Nanotube Polymers. ACS Nano, 2011, 5, 7226-7234.	7.3	110
11	Potential high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:ma superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaYH</mml:mi><mml:mn>12</mml:mn></mml:msub> under pressure. Physical Review B, 2019, 99, .	1.1	109
12	Two-dimensional magnetic boron. Physical Review B, 2016, 93, .	1.1	101
13	Tuning the catalytic property of nitrogen-doped graphene for cathode oxygen reduction reaction. Physical Review B, 2012, 85, .	1.1	81
14	Variable cell nudged elastic band method for studying solidâ€“solid structural phase transitions. Computer Physics Communications, 2013, 184, 2111-2118.	3.0	71
15	Most likely phase of superhard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>BC</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>byab initiocalculations. Physical Review B, 2007, 76, .	1.1	62
16	New Reconstructions of the (110) Surface of Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:m by an Evolutionary Method. Physical Review Letters, 2014, 113, 266101.	2.9	61
17	Origin of insulating behavior of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaAlO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Polarization-induced asymmetric distribution of oxygen va. Physical Review B, 2010, 82, .	1.1	59
18	Blackâ€Phosphorusâ€Based Orientationâ€Induced Diodes. Advanced Materials, 2018, 30, 1704653.	11.1	53

#	ARTICLE	IF	CITATIONS
19	Discovery of carbon-based strongest and hardest amorphous material. National Science Review, 2022, 9, nwab140.	4.6	49
20	Superconducting high-pressure phase of platinum hydride from first principles. Physical Review B, 2011, 84, .	1.1	47
21	First-Principles Determination of the Structure of Magnesium Borohydride. Physical Review Letters, 2012, 109, 245503.	2.9	47
22	Bulk Re₂C: Crystal Structure, Hardness, and Ultra-incompressibility. Crystal Growth and Design, 2010, 10, 5024-5026.	1.4	46
23	Chalcopyrite polymorph for superhard BC2N. Applied Physics Letters, 2006, 89, 151911.	1.5	41
24	Crystal structure and stability of magnesium borohydride from first principles. Physical Review B, 2009, 79, .	1.1	39
25	Superconductivity of novel tin hydrides (SnnHm) under pressure. Scientific Reports, 2016, 6, 22873.	1.6	39
26	Refined Crystal Structure and Mechanical Properties of Superhard BC₄N Crystal: First-Principles Calculations. Journal of Physical Chemistry C, 2008, 112, 9516-9519.	1.5	38
27	First-principles study of crystal structures and superconductivity of ternary <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YSH</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaSH</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math> at high pressures. Physical Review B, 2019, 100, .	1.1	33
28	A tetragonal phase of superhard BC2N. Journal of Applied Physics, 2009, 105, .	1.1	32
29	Continuous strengthening in nanotwinned diamond. Npj Computational Materials, 2019, 5, .	3.5	32
30	Prediction of a new ground state of superhard compound B6O at ambient conditions. Scientific Reports, 2016, 6, 31288.	1.6	31
31	Mechanical properties of boron arsenide single crystal. Applied Physics Letters, 2019, 114, .	1.5	31
32	Unexpected Reconstruction of theÎ±-Boron (111) Surface. Physical Review Letters, 2014, 113, 176101.	2.9	29
33	Unusual compression behavior of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> from first principles. Physical Review B, 2010, 82, .	1.1	28
34	High-pressure behaviors of carbon nanotubes. Journal of Superhard Materials, 2012, 34, 371-385.	0.5	28
35	Predicting the ground-state structure of sodium boride. Physical Review B, 2018, 97, .	1.1	26
36	Magnetic borophenes from an evolutionary search. Physical Review B, 2019, 99, .	1.1	25

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37	Electronegativity and chemical hardness of elements under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2117416119.	3.3	25
38	An ab initio study on the transition paths from graphite to diamond under pressure. Journal of Physics Condensed Matter, 2013, 25, 145402.	0.7	22
39	Predicting three-dimensional icosahedron-based boron <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>. Physical Review B, 2019, 99, .	1.1	21
40	Boron oxides under pressure: Prediction of the hardest oxides. Physical Review B, 2018, 98, .	1.1	18
41	Infrared and Raman spectra ofÎ²â€²BC2Nfrom first principles calculations. Physical Review B, 2006, 74, .	1.1	17
42	Formation, structure, and electric property of CaB4 single crystal synthesized under high pressure. Applied Physics Letters, 2010, 96, .	1.5	17
43	Novel superhard boron-rich nitrides under pressure. Science China Materials, 2020, 63, 2358-2364.	3.5	17
44	Si₁₀: A sp³ Silicon Allotrope with Spirally Connected Si₅ Tetrahedrons. Chemistry of Materials, 2016, 28, 6441-6445.	3.2	16
45	Helium-nitrogen mixtures at high pressure. Physical Review B, 2021, 103, .	1.1	16
46	Ultrahigh-Pressure Magnesium Hydrosilicates as Reservoirs of Water in Early Earth. Physical Review Letters, 2022, 128, 035703.	2.9	16
47	High-pressure phases of boron arsenide with potential high thermal conductivity. Physical Review B, 2019, 99, .	1.1	15
48	Small onion-like BN leads to ultrafine-twinned cubic BN. Science China Materials, 2019, 62, 1169-1176.	3.5	15
49	Formation of copper boride on Cu(111). Fundamental Research, 2021, 1, 482-487.	1.6	15
50	Low-dimensional boron: searching for Dirac materials. Advances in Physics: X, 2016, 1, 412-424.	1.5	14
51	Crystal Structure Prediction and Its Application in Earth and Materials Sciences. Topics in Current Chemistry, 2014, 345, 223-256.	4.0	12
52	Prediction of superconductivity in pressure-induced new silicon boride phases. Physical Review B, 2020, 101, .	1.1	12
53	Universal Phase Transitions of B1-Structured Stoichiometric Transition Metal Carbides. Inorganic Chemistry, 2011, 50, 9266-9272.	1.9	11
54	A novel phase of beryllium fluoride at high pressure. Physical Chemistry Chemical Physics, 2015, 17, 26283-26288.	1.3	11

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55	Large shear strength enhancement of gamma-boron by normal compression. Journal of Superhard Materials, 2011, 33, 401-408.	0.5	10
56	Highâ€pressure phases of NaAlH4 from first principles. Applied Physics Letters, 2012, 100, 061905.	1.5	10
57	Novel magnesium borides and their superconductivity. Physical Chemistry Chemical Physics, 2017, 19, 14486-14494.	1.3	10
58	Nitrogen oxides under pressure: stability, ionization, polymerization and superconductivity. Scientific Reports, 2015, 5, 16311.	1.6	9
59	Photoinduced Orientationâ€Dependent Interlayer Carrier Transportation in Crossâ€Stacked Black Phosphorus van der Waals Junctions. Advanced Materials Interfaces, 2018, 5, 1800964.	1.9	8
60	First-principles prediction of two-dimensional copper borides. Physical Review Materials, 2020, 4, .	0.9	8
61	Low-energy 3D sp²carbons with versatile properties beyond graphite and graphene. Dalton Transactions, 2018, 47, 6233-6239.	1.6	7
62	Two-dimensional boron on Pb (1 1 0) surface. FlatChem, 2018, 7, 34-41.	2.8	7
63	Predicted lithium oxide compounds and superconducting low-pressure <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiO</mml:mi><mml:mn>4</mml:mn></mml:msub></m Physical Review B, 2019, 100, .	1.1	7
64	Superconductivity in graphite-diamond hybrid. Materials Today Physics, 2022, 23, 100630.	2.9	7
65	Phase transition of layer-stacked borophene under pressure. Physical Review B, 2022, 105, .	1.1	5
66	Negative linear compressibility and unusual dynamic behavior of NaB3. Physical Review Materials, 2021, 5, .	0.9	1