Xiang-Feng Zhou

List of Publications by Citations

65 papers	4,252 citations	27 h-index	65 g-index
68 ext. papers	5,017 ext. citations	6.4 avg, IF	5.16 L-index

#	Paper	IF	Citations
65	Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs. *Science*, **2015**, 350, 1513-6	33.3	1479
64	Semimetallic Two-Dimensional Boron Allotrope with Massless Dirac Fermions. *Physical Review Letters*, **2014**, 112,	7.4	397
63	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. *Nano Letters*, **2015**, 15, 6182-6	11.5	325
62	A stable compound of helium and sodium at high pressure. *Nature Chemistry*, **2017**, 9, 440-445	17.6	199
61	Novel superhard carbon: C-centered orthorhombic C8. *Physical Review Letters*, **2011**, 107, 215502	7.4	198
60	Strain effects on borophene: ideal strength, negative Possion□ ratio and phonon instability. *New Journal of Physics*, **2016**, 18, 073016	2.9	141
59	Ab initio study of the formation of transparent carbon under pressure. *Physical Review B*, **2010**, 82,	3.3	108
58	Three dimensional carbon-nanotube polymers. *ACS Nano*, **2011**, 5, 7226-34	16.7	94
57	First-principles study of electronic structure and optical properties of heterodiamond BC2N. *Physical Review B*, **2006**, 73,	3.3	91
56	Two-dimensional magnetic boron. *Physical Review B*, **2016**, 93,	3.3	75
55	Tuning the catalytic property of nitrogen-doped graphene for cathode oxygen reduction reaction. *Physical Review B*, **2012**, 85,	3.3	69
54	Hierarchically structured diamond composite with exceptional toughness. *Nature*, **2020**, 582, 370-374	50.4	59
53	Variable cell nudged elastic band method for studying solid□solid structural phase transitions. *Computer Physics Communications*, **2013**, 184, 2111-2118	4.2	56
52	Most likely phase of superhard BC2N by ab initio calculations. *Physical Review B*, **2007**, 76,	3.3	54
51	Potential high-Tc superconductivity in CaYH12 under pressure. *Physical Review B*, **2019**, 99,	3.3	53
50	Origin of insulating behavior of the p-type LaAlO3/SrTiO3 interface: Polarization-induced asymmetric distribution of oxygen vacancies. *Physical Review B*, **2010**, 82,	3.3	53
49	New reconstructions of the (110) surface of rutile TiO2 predicted by an evolutionary method. *Physical Review Letters*, **2014**, 113, 266101	7.4	50

48	First-principles determination of the structure of magnesium borohydride. *Physical Review Letters*, **2012**, 109, 245503	7.4	43
47	Superconducting high-pressure phase of platinum hydride from first principles. *Physical Review B*, **2011**, 84,	3.3	43
46	Bulk Re2C: Crystal Structure, Hardness, and Ultra-incompressibility. *Crystal Growth and Design*, **2010**, 10, 5024-5026	3.5	40
45	Black-Phosphorus-Based Orientation-Induced Diodes. *Advanced Materials*, **2018**, 30, 1704653	24	38
44	Crystal structure and stability of magnesium borohydride from first principles. *Physical Review B*, **2009**, 79,	3.3	37
43	Chalcopyrite polymorph for superhard BC2N. *Applied Physics Letters*, **2006**, 89, 151911	3.4	37
42	Refined Crystal Structure and Mechanical Properties of Superhard BC4N Crystal: First-Principles Calculations. *Journal of Physical Chemistry C*, **2008**, 112, 9516-9519	3.8	32
41	Superconductivity of novel tin hydrides (Sn(n)H(m)) under pressure. *Scientific Reports*, **2016**, 6, 22873	4.9	29
40	A tetragonal phase of superhard BC2N. *Journal of Applied Physics*, **2009**, 105, 093521	2.5	28
39	Unusual compression behavior of TiO2 polymorphs from first principles. *Physical Review B*, **2010**, 82,	3.3	27
38	Prediction of a new ground state of superhard compound B6O at ambient conditions. *Scientific Reports*, **2016**, 6, 31288	4.9	26
37	Unexpected reconstruction of the □boron (111) surface. *Physical Review Letters*, **2014**, 113, 176101	7.4	26
36	High-pressure behaviors of carbon nanotubes. *Journal of Superhard Materials*, **2012**, 34, 371-385	0.9	22
35	Formation, structure, and electric property of CaB4 single crystal synthesized under high pressure. *Applied Physics Letters*, **2010**, 96, 031903	3.4	17
34	Continuous strengthening in nanotwinned diamond. *Npj Computational Materials*, **2019**, 5,	10.9	17
33	Predicting the ground-state structure of sodium boride. *Physical Review B*, **2018**, 97,	3.3	16
32	First-principles study of crystal structures and superconductivity of ternary YSH6 and LaSH6 at high pressures. *Physical Review B*, **2019**, 100,	3.3	16
31	Discovery of carbon-based strongest and hardest amorphous material.. *National Science Review*, **2022**, 9, nwab140	10.8	16

30	Predicting three-dimensional icosahedron-based boron B60. *Physical Review B*, **2019**, 99,	3.3	15
29	Magnetic borophenes from an evolutionary search. *Physical Review B*, **2019**, 99,	3.3	15
28	Mechanical properties of boron arsenide single crystal. *Applied Physics Letters*, **2019**, 114, 131903	3.4	15
27	Infrared and Raman spectra of **B**C2N from first principles calculations. *Physical Review B*, **2006**, 74,	3.3	15
26	Si10: A sp3 Silicon Allotrope with Spirally Connected Si5 Tetrahedrons. *Chemistry of Materials*, **2016**, 28, 6441-6445	9.6	14
25	An ab initio study on the transition paths from graphite to diamond under pressure. *Journal of Physics Condensed Matter*, **2013**, 25, 145402	1.8	13
24	Boron oxides under pressure: Prediction of the hardest oxides. *Physical Review B*, **2018**, 98,	3.3	13
23	Low-dimensional boron: searching for Dirac materials. *Advances in Physics: X*, **2016**, 1, 412-424	5.1	12
22	High-pressure phases of boron arsenide with potential high thermal conductivity. *Physical Review B*, **2019**, 99,	3.3	11
21	Universal phase transitions of B1-structured stoichiometric transition metal carbides. *Inorganic Chemistry*, **2011**, 50, 9266-72	5.1	11
20	A novel phase of beryllium fluoride at high pressure. *Physical Chemistry Chemical Physics*, **2015**, 17, 26283-8	3.6	10
19	Crystal structure prediction and its application in Earth and materials sciences. *Topics in Current Chemistry*, **2014**, 345, 223-56		10
18	Small onion-like BN leads to ultrafine-twinned cubic BN. *Science China Materials*, **2019**, 62, 1169-1176	7.1	9
17	Large shear strength enhancement of gamma-boron by normal compression. *Journal of Superhard Materials*, **2011**, 33, 401-408	0.9	9
16	Nitrogen oxides under pressure: stability, ionization, polymerization, and superconductivity. *Scientific Reports*, **2015**, 5, 16311	4.9	8
15	High-pressure phases of NaAlH4 from first principles. *Applied Physics Letters*, **2012**, 100, 061905	3.4	8
14	Novel superhard boron-rich nitrides under pressure. *Science China Materials*, **2020**, 63, 2358-2364	7.1	7
13	Novel magnesium borides and their superconductivity. *Physical Chemistry Chemical Physics*, **2017**, 19, 14486-14494	3.6	6

12	Low-energy 3D sp carbons with versatile properties beyond graphite and graphene. *Dalton Transactions*, **2018**, 47, 6233-6239	4.3	6
11	Two-dimensional boron on Pb (1 1 0) surface. *FlatChem*, **2018**, 7, 34-41	5.1	5
10	Photoinduced Orientation-Dependent Interlayer Carrier Transportation in Cross-Stacked Black Phosphorus van der Waals Junctions. *Advanced Materials Interfaces*, **2018**, 5, 1800964	4.6	5
9	Prediction of superconductivity in pressure-induced new silicon boride phases. *Physical Review B*, **2020**, 101,	3.3	4
8	First-principles prediction of two-dimensional copper borides. *Physical Review Materials*, **2020**, 4,	3.2	4
7	Ultrahigh-Pressure Magnesium Hydrosilicates as Reservoirs of Water in Early Earth.. *Physical Review Letters*, **2022**, 128, 035703	7.4	3
6	Helium-nitrogen mixtures at high pressure. *Physical Review B*, **2021**, 103,	3.3	3
5	Electronegativity and chemical hardness of elements under pressure.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2117416119	11.5	3
4	Predicted lithium oxide compounds and superconducting low-pressure LiO4. *Physical Review B*, **2019**, 100,	3.3	2
3	Superconductivity in graphite-diamond hybrid. *Materials Today Physics*, **2022**, 23, 100630	8	2
2	Formation of copper boride on Cu(111). *Fundamental Research*, **2021**, 1, 482-487		2
1	Predicting the Structure and Chemistry of Low-Dimensional Materials **2017**, 527-570		