Changfeng Chen

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138 papers	6,187 citations	38 h-index	75 g-index
151 ext. papers	7,120 ext. citations	5.5 avg, IF	6.48 L-index

#	Paper	IF	Citations
138	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct I-V Response. *Journal of Physical Chemistry Letters*, **2014**, 5, 2675-81	6.4	723
137	Phosphorene: Fabrication, Properties, and Applications. *Journal of Physical Chemistry Letters*, **2015**, 6, 2794-805	6.4	545
136	Global structural optimization of tungsten borides. *Physical Review Letters*, **2013**, 110, 136403	7.4	216
135	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS2 Nanoribbons. *Journal of Physical Chemistry Letters*, **2012**, 3, 2934-41	6.4	203
134	Harder than diamond: superior indentation strength of wurtzite BN and lonsdaleite. *Physical Review Letters*, **2009**, 102, 055503	7.4	196
133	Thermodynamic properties of PbTe, PbSe, and PbS: First-principles study. *Physical Review B*, **2009**, 80,	3.3	196
132	Superhard cubic BC2N compared to diamond. *Physical Review Letters*, **2004**, 93, 195504	7.4	184
131	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147
130	Body-Centered Orthorhombic C_{16}: A Novel Topological Node-Line Semimetal. *Physical Review Letters*, **2016**, 116, 195501	7.4	129
129	Is osmium diboride an ultra-hard material?. *Journal of the American Chemical Society*, **2008**, 130, 7200-1	16.4	127
128	Nanoscale Multilayer Transition-Metal Dichalcogenide Heterostructures: Band Gap Modulation by Interfacial Strain and Spontaneous Polarization. *Journal of Physical Chemistry Letters*, **2013**, 4, 1730-6	6.4	126
127	Auxetic and Ferroelastic Borophane: A Novel 2D Material with Negative Possion's Ratio and Switchable Dirac Transport Channels. *Nano Letters*, **2016**, 16, 7910-7914	11.5	121
126	Two-Dimensional Topological Insulators: Progress and Prospects. *Journal of Physical Chemistry Letters*, **2017**, 8, 1905-1919	6.4	110
125	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. *Physical Review Letters*, **2017**, 119, 115503	7.4	108
124	Modifying atomic-scale friction between two graphene sheets: A molecular-force-field study. *Physical Review B*, **2007**, 76,	3.3	107
123	Structural deformation, strength, and instability of cubic BN compared to diamond: A first-principles study. *Physical Review B*, **2006**, 73,	3.3	106
122	Atomistic deformation modes in strong covalent solids. *Physical Review Letters*, **2005**, 94, 145505	7.4	104

121	Anisotropic Ripple Deformation in Phosphorene. *Journal of Physical Chemistry Letters*, **2015**, 6, 1509-13	6.4	88
120	Tuning field-induced energy gap of bilayer graphene via interlayer spacing. *Applied Physics Letters*, **2008**, 92, 243101	3.4	86
119	Anomalous Stress Response of Ultrahard WB_{n} Compounds. *Physical Review Letters*, **2015**, 115, 185502	7.4	85
118	Orthorhombic carbon allotrope of compressed graphite: Ab initio calculations. *Physical Review B*, **2012**, 85,	3.3	75
117	Photoelectron Spectra and Geometric Structures of Small Niobium Cluster Anions. *Physical Review Letters*, **1996**, 77, 4528-4531	7.4	75
116	Large indentation strain-stiffening in nanotwinned cubic boron nitride. *Nature Communications*, **2014**, 5, 4965	17.4	74
115	Topological Nodal-Net Semimetal in a Graphene Network Structure. *Physical Review Letters*, **2018**, 120, 026402	7.4	68
114	A new carbon allotrope with six-fold helical chains in all-sp2 bonding networks. *Scientific Reports*, **2014**, 4, 4339	4.9	67
113	Colossal shear-strength enhancement of low-density cubic BC2N by nanoindentation. *Physical Review Letters*, **2007**, 98, 135505	7.4	64
112	High-Pressure Evolution of Crystal Bonding Structures and Properties of FeOOH. *Journal of Physical Chemistry Letters*, **2018**, 9, 2181-2185	6.4	57
111	Extreme Mechanics of Probing the Ultimate Strength of Nanotwinned Diamond. *Physical Review Letters*, **2016**, 117, 116103	7.4	52
110	Unraveling the structure and bonding evolution of the newly discovered iron oxide FeO2. *Physical Review B*, **2018**, 98,	3.3	51
109	Strain dependent bonding in solid C3N4: High elastic moduli but low strength. *Physical Review B*, **2006**, 73,	3.3	50
108	Elucidating Stress-Strain Relations of ZrB from First-Principles Studies. *Journal of Physical Chemistry Letters*, **2020**, 11, 9165-9170	6.4	50
107	Soft bond-deformation paths in superhard □boron. *Physical Review Letters*, **2010**, 105, 215503	7.4	49
106	Molecular dynamics simulation of tensile elongation of carbon nanotubes: Temperature and size effects. *Physical Review B*, **2009**, 79,	3.3	45
105	Interplay of Dirac electrons and magnetism in CaMnBi and SrMnBi. *Nature Communications*, **2016**, 7, 13833	17.4	45
104	Ultralow-Frequency Collective Compression Mode and Strong Interlayer Coupling in Multilayer Black Phosphorus. *Physical Review Letters*, **2016**, 116, 087401	7.4	42

103	Unexpectedly low indentation strength of WB3 and MoB3 from first principles. *Physical Review B*, **2012**, 86,	3.3	42
102	CoB6 monolayer: A robust two-dimensional ferromagnet. *Physical Review B*, **2019**, 99,	3.3	42
101	Indentation strength of ultraincompressible rhenium boride, carbide, and nitride from first-principles calculations. *Physical Review B*, **2012**, 86,	3.3	41
100	Rare Helium-Bearing Compound FeO_{2}He Stabilized at Deep-Earth Conditions. *Physical Review Letters*, **2018**, 121, 255703	7.4	38
99	Computational prediction of body-centered cubic carbon in an all-sp3 six-member ring configuration. *Physical Review B*, **2015**, 91,	3.3	37
98	Structure-strength relations of distinct MoN phases from first-principles calculations. *Physical Review Materials*, **2020**, 4,	3.2	36
97	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. *Journal of Physical Chemistry C*, **2013**, 117, 5352-5357	3.8	35
96	Fundamental constraints on the strength of transition-metal borides: The case of CrB4. *Physical Review B*, **2013**, 87,	3.3	35
95	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. *Physical Review Materials*, **2020**, 4,	3.2	35
94	Superconductivity in Compression-Shear Deformed Diamond. *Physical Review Letters*, **2020**, 124, 147001	7.4	33
93	First-principles calculation of the indentation strength of FeB4. *Physical Review B*, **2014**, 90,	3.3	32
92	Mechanism for direct conversion of graphite to diamond. *Physical Review B*, **2011**, 84,	3.3	32
91	Indentation Strengths of Zirconium Diboride: Intrinsic versus Extrinsic Mechanisms. *Journal of Physical Chemistry Letters*, **2021**, 12, 2848-2853	6.4	32
90	Aspect ratio dependent buckling mode transition in single-walled carbon nanotubes under compression. *Journal of Applied Physics*, **2011**, 109, 084323	2.5	31
89	Controllable CO electrocatalytic reduction via ferroelectric switching on single atom anchored InSe monolayer. *Nature Communications*, **2021**, 12, 5128	17.4	30
88	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. *ACS Applied Materials & Interfaces*, **2015**, 7, 19226-33	9.5	28
87	New carbon allotropes in sp + sp bonding networks consisting of C cubes. *Physical Chemistry Chemical Physics*, **2018**, 20, 7962-7967	3.6	27
86	Multiferroic and Ferroic Topological Order in Ligand-Functionalized Germanene and Arsenene. *Physical Review Applied*, **2018**, 10,	4.3	27

85	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. *Physical Review Letters*, **2019**, 123, 195504	7.4	27
84	Phase stability of carbon clathrates at high pressure. *Journal of Applied Physics*, **2010**, 107, 063507	2.5	27
83	Tuning the magnetic and electronic properties of bilayer graphene nanoribbons on Si(001) by bias voltage. *Physical Review B*, **2010**, 81,	3.3	27
82	Thermodynamic functions and pressure-temperature phase diagram of lithium alanates by ab initio calculations. *Physical Review B*, **2007**, 76,	3.3	27
81	Ideal tensile and shear strength of □3N4 from first-principles calculations. *Physical Review B*, **2007**, 76,	3.3	27
80	Two-dimensional ferroelectric topological insulators in functionalized atomically thin bismuth layers. *Physical Review B*, **2018**, 97,	3.3	26
79	Tetragonal crystalline carbon nitrides: theoretical predictions. *Physical Review Letters*, **2001**, 86, 652-5	7.4	26
78	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp(2) Hybrid Networks. *Scientific Reports*, **2016**, 6, 24665	4.9	25
77	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. *Journal of Physical Chemistry C* , **2013**, 117, 12266-12271	3.8	24
76	New cubic carbon phase via graphitic sheet rumpling. *Physical Review B*, **2012**, 85,	3.3	23
75	Structural and mechanical properties of partially unzipped carbon nanotubes. *Physical Review B*, **2011**, 83,	3.3	23
74	Diverging synthesis routes and distinct properties of cubic BC2N at high pressure. *Physical Review B* , **2004**, 70,	3.3	23
73	Chemically Tuning Stability and Superconductivity of P-H Compounds. *Journal of Physical Chemistry Letters*, **2020**, 11, 935-939	6.4	21
72	Ideal strength and structural instability of aluminum at finite temperatures. *Physical Review B*, **2012** , 86,	3.3	21
71	Transition from band insulator to Mott insulator in one dimension: Critical behavior and phase diagram. *Physical Review B*, **2003**, 68,	3.3	21
70	Structural metatransition of energetically tangled crystalline phases. *Physical Chemistry Chemical Physics*, **2017**, 19, 4560-4566	3.6	20
69	Interlayer stacking and nature of the electronic band gap in graphitic BC2N: First-principles pseudopotential calculations. *Physical Review B*, **2006**, 73,	3.3	20
68	Topological nodal line semimetal in an orthorhombic graphene network structure. *Physical Review B*, **2018**, 97,	3.3	20

67	Charge carrier separation induced by intrinsic surface strain in pristine ZnO nanowires. *Applied Physics Letters*, **2010**, 97, 053104	3.4	19
66	Highly stable and symmetric boron caged B@Co12@B80 core-shell cluster. *Applied Physics Letters*, **2009**, 94, 133102	3.4	19
65	Field-induced gap in the spin-12 antiferromagnetic Heisenberg chain: A density-matrix renormalization-group study. *Physical Review B*, **2002**, 65,	3.3	19
64	Indenter-angle-sensitive fracture modes and stress response at incipient plasticity. *Physical Review B*, **2009**, 79,	3.3	18
63	Computational discovery of a new rhombohedral diamond phase. *Physical Review B*, **2018**, 98,	3.3	18
62	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. *Journal of Physical Chemistry Letters*, **2019**, 10, 2761-2766	6.4	17
61	Multiferroic decorated FeO monolayer predicted from first principles. *Nanoscale*, **2020**, 12, 14847-14852	7.7	16
60	Unravelling the structure and strength of the highest boride of tungsten WB4.2. *Physical Review B*, **2019**, 100,	3.3	16
59	Ab initio prediction of superdense tetragonal and monoclinic polymorphs of carbon. *Physical Review B*, **2016**, 94,	3.3	15
58	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. *Journal of Physical Chemistry C*, **2013**, 117, 8437-8442	3.8	15
57	Ab initio structural identification of high density cubic BC2N. *Physical Review B*, **2006**, 73,	3.3	15
56	Bias voltage induced n- to p-type transition in epitaxial bilayer graphene on SiC. *Physical Review B*, **2009**, 80,	3.3	14
55	Local-Strain-Induced Charge Carrier Separation and Electronic Structure Modulation in Zigzag ZnO Nanotubes: Role of Built-In Polarization Electric Field. *Journal of Physical Chemistry C*, **2011**, 115, 2381-2385	3.8	13
54	Tuning Magnetism of Metal Porphyrazine Molecules by a Ferroelectric InSe Monolayer. *ACS Applied Materials & Interfaces*, **2020**, 12, 39561-39566	9.5	13
53	Kondo Signatures of a Quantum Magnetic Impurity in Topological Superconductors. *Physical Review Letters*, **2019**, 122, 087001	7.4	12
52	High-mobility anisotropic transport in few-layer □B films. *Nanoscale*, **2016**, 8, 20111-20117	7.7	12
51	Intrinsic Charge Separation and Tunable Electronic Band Gap of Armchair Graphene Nanoribbons Encapsulated in a Double-Walled Carbon Nanotube. *Journal of Physical Chemistry Letters*, **2013**, 4, 1328-33	6.4	12
50	Hybrid W-shaped graphene nanoribbons: Distinct electronic and transport properties. *Journal of Applied Physics*, **2011**, 110, 124312	2.5	12

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48	Three-Dimensional Crystalline Modification of Graphene in all-sp Hexagonal Lattices with or without Topological Nodal Lines. *Journal of Physical Chemistry Letters*, **2019**, 10, 2515-2521	6.4	11
47	Thermoelectric properties of rocksalt ZnO from first-principles calculations. *Journal of Applied Physics*, **2015**, 118, 165101	2.5	11
46	Enhancing interwall load transfer by vacancy defects in carbon nanotubes. *Applied Physics Letters*, **2012**, 100, 033118	3.4	11
45	NOVEL MANY-BODY EFFECTS IN PHOTOEMISSION AND INVERSE PHOTOEMISSION SPECTRA OF ULTRATHIN TRANSITION-METAL FILMS. *International Journal of Modern Physics B*, **1991**, 05, 1147-1178	1.1	11
44	Superior magnetic and mechanical property of MnFe3N driven by electron correlation and lattice anharmonicity. *Physical Review B*, **2015**, 91,	3.3	10
43	Ground-state phase diagram of a spin-12 frustrated three-leg antiferromagnetic Heisenberg ladder. *Physical Review B*, **2002**, 66,	3.3	10
42	Body centered cubic carbon BC14: An all-sp3 bonded full-fledged pentadiamond. *Physical Review B*, **2020**, 102,	3.3	10
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40	Ab initio study of the anharmonic lattice dynamics of iron at the □phase transition. *Physical Review B*, **2015**, 92,	3.3	9
39	Anomalous strength anisotropy of □-Fe4N identified by first-principles calculations. *Applied Physics Letters*, **2009**, 94, 151914	3.4	9
38	Stability of HO at extreme conditions and implications for the magnetic fields of Uranus and Neptune. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 5638-5643	11.5	8
37	Topological semimetal in an sp2□sp3 hybridized carbon network with nodal rings. *Physical Review B* , **2020**, 101,	3.3	8
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35	Intrinsic low thermal conductivity in weakly ionic rocksalt structures. *Physical Review B*, **2015**, 92,	3.3	8
34	Sorting transition-metal diborides: New descriptor for mechanical properties. *Acta Materialia*, **2021**, 207, 116685	8.4	8
33	Unexpected structural softening of interstitial boron solid solution WB3+x. *Applied Physics Letters*, **2014**, 105, 211901	3.4	7
32	First-principles prediction of low-energy structures for AlH3. *Physical Review B*, **2009**, 79,	3.3	7

31	Excitons in spatially separated electron–hole systems: A quantum Monte Carlo study. *Journal of Applied Physics*, **1995**, 78, 7099-7102	2.5	7
30	Structural and electronic phase transitions of ThS2 from first-principles calculations. *Physical Review B*, **2016**, 94,	3.3	7
29	Phase stability and transition of BaSi2-type disilicides and digermanides. *Physical Review B*, **2015**, 91,	3.3	6
28	Probing the direct factor for superconductivity in FeSe-Based Superconductors by Raman Scattering. *Physical Review B*, **2019**, 100,	3.3	6
27	Topological nodal line semimetals in graphene network structures. *Advances in Physics: X*, **2019**, 4, 1625724	3.4	6
26	Antiferromagnetic Heisenberg ladders in staggered magnetic field. *Physical Review B*, **2006**, 73,	3.3	6
25	Xenon iron oxides predicted as potential Xe hosts in Earth's lower mantle. *Nature Communications*, **2020**, 11, 5227	17.4	6
24	Robust Magnetoelectric Effect in the Decorated Graphene/InSe Heterostructure. *ACS Applied Materials & Interfaces*, **2021**, 13, 3033-3039	9.5	6
23	Superconductivity in Shear Strained Semiconductors. *Chinese Physics Letters*, **2021**, 38, 086301	1.8	5
22	Extreme static compression of carbon to terapascal pressures. *Carbon*, **2019**, 144, 161-170	10.4	5
21	Pronounced Enhancement of Superconductivity in ZrN via Strain Engineering. *Journal of Physical Chemistry Letters*, **2021**, 12, 1985-1990	6.4	5
20	Phonon-mediated high-T superconductivity in hole-doped diamond-like crystalline hydrocarbon. *Scientific Reports*, **2017**, 7, 1464	4.9	4
19	Tunable quantum order in bilayer Bi2Te3: Stacking dependent quantum spin Hall states. *Applied Physics Letters*, **2018**, 112, 243103	3.4	4
18	Pressure-constrained deformation and superior strength: Compressed graphite versus diamond. *Physical Review B*, **2013**, 88,	3.3	4
17	First-principles study of high-pressure phase stability and superconductivity of Bi4I4. *Physical Review B*, **2019**, 100,	3.3	4
16	Surface Concavity–Convexity Sensitive Oxidation Dynamics of Carbon Nanotubes. *Journal of Physical Chemistry C*, **2009**, 113, 3569-3573	3.8	3
15	Effect of strain on the energetics and kinetics of dissociation of Sb4 on Ge(001). *Physical Review B*, **2008**, 78,	3.3	3
14	On the Characteristics of the Pseudogapped Metallic State of High-Tc Superconductors. *International Journal of Modern Physics B*, **1998**, 12, 3052-3056	1.1	3

13	Atomistic Mechanisms for Contrasting Stress-Strain Relations of BCN and BC. *Journal of Physical Chemistry Letters*, **2020**, 11, 10454-10462	6.4	3
12	Pressure-stabilized divalent ozonide CaO and its impact on Earth's oxygen cycles. *Nature Communications*, **2020**, 11, 4702	17.4	3
11	Reply to "Anisotropy governs strain stiffening in nanotwinned-materials". *Nature Communications*, **2018**, 9, 1585	17.4	2
10	Buckling of double-walled carbon nanotubes under compression and bending: Influence of vacancy defects and effect of high-temperature annealing. *Journal of Applied Physics*, **2013**, 114, 174308	2.5	2
9	Structural Relaxation of Vacancies in Amorphous Silicon. *Materials Research Society Symposia Proceedings*, **1997**, 467, 555		2
8	Buckling of blue phosphorus nanotubes under axial compression: Insights from molecular dynamics simulations. *Journal of Applied Physics*, **2020**, 127, 014301	2.5	2
7	Toughening a superstrong carbon crystal: Sequential bond-breaking mechanisms. *Physical Review B*, **2020**, 102,	3.3	2
6	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. *Journal of Physical Chemistry Letters*, **2021**, 12, 2036-2043	6.4	2
5	Pentagraphite C8 : An all- sp2 topological nodal-line semimetal. *Physical Review B*, **2021**, 104,	3.3	2
4	New carbon allotropes derived from nanotubes via a three-fold distortion mechanism. *Physical Chemistry Chemical Physics*, **2020**, 22, 12489-12495	3.6	1
3	Macroscale Robust Superlubricity on Metallic NbB.. *Advanced Science*, **2022**, e2103815	13.6	0
2	Structural Characterization of Crystalline Si-C-N Films. *Materials Research Society Symposia Proceedings*, **1997**, 498, 301		
1	Exact Diagonalization Study of Real Materials. *Materials Research Society Symposia Proceedings*, **1992**, 291, 253		