

Changfeng Chen

List of Publications by Year in descending order

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papers

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57719

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docs citations

151
times ranked

7602
citing authors

#	ARTICLE	IF	CITATIONS
1	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct $\Delta I/I_0$ Response. Journal of Physical Chemistry Letters, 2014, 5, 2675-2681.	2.1	877
2	Phosphorene: Fabrication, Properties, and Applications. Journal of Physical Chemistry Letters, 2015, 6, 2794-2805.	2.1	680
3	Global Structural Optimization of Tungsten Borides. Physical Review Letters, 2013, 110, 136403.	2.9	253
4	Harder than Diamond: Superior Indentation Strength of Wurtzite BN and Lonsdaleite. Physical Review Letters, 2009, 102, 055503.	2.9	250
5	Thermodynamic properties of PbTe, PbSe, and PbS: First-principles study. Physical Review B, 2009, 80, .	1.1	231
6	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS ₂ Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 2934-2941.	2.1	229
7	Superhard Cubic BC ₂ N Compared to Diamond. Physical Review Letters, 2004, 93, 195504.	2.9	214
8	Superhard BC_3 Cubic Diamond Structure. Physical Review Letters, 2015, 114, 015502.	2.9	180
9	Auxetic and Ferroelastic Borophane: A Novel 2D Material with Negative Poisson's Ratio and Switchable Dirac Transport Channels. Nano Letters, 2016, 16, 7910-7914.	4.5	176
10	Body-Centered Orthorhombic C_{16} A Novel Topological Node-Line Semimetal. Physical Review Letters, 2016, 116, 195501.	2.9	170
11	Two-Dimensional Topological Insulators: Progress and Prospects. Journal of Physical Chemistry Letters, 2017, 8, 1905-1919.	2.1	170
12	Nanoscale Multilayer Transition-Metal Dichalcogenide Heterostructures: Band Gap Modulation by Interfacial Strain and Spontaneous Polarization. Journal of Physical Chemistry Letters, 2013, 4, 1730-1736.	2.1	142
13	Is Osmium Diboride An Ultra-Hard Material?. Journal of the American Chemical Society, 2008, 130, 7200-7201.	6.6	132
14	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. Physical Review Letters, 2017, 119, 115503.	2.9	129
15	Modifying atomic-scale friction between two graphene sheets: A molecular-force-field study. Physical Review B, 2007, 76, .	1.1	127
16	Structural deformation, strength, and instability of cubic BN compared to diamond: A first-principles study. Physical Review B, 2006, 73, .	1.1	125
17	Atomistic Deformation Modes in Strong Covalent Solids. Physical Review Letters, 2005, 94, 145505.	2.9	119
18	Controllable CO ₂ electrocatalytic reduction via ferroelectric switching on single atom anchored In ₂ Se ₃ monolayer. Nature Communications, 2021, 12, 5128.	5.8	110

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19	Anomalous Stress Response of Ultrahard $W\text{B}_n$. Physical Review Letters, 2015, 115, 185502.	2.9	107
20	Anisotropic Ripple Deformation in Phosphorene. Journal of Physical Chemistry Letters, 2015, 6, 1509-1513.	2.1	106
21	Large indentation strain-stiffening in nanotwinned cubic boron nitride. Nature Communications, 2014, 5, 4965.	5.8	105
22	Elucidating Stress-Strain Relations of ZrB_{12} from First-Principles Studies. Journal of Physical Chemistry Letters, 2020, 11, 9165-9170.	2.1	97
23	Tuning field-induced energy gap of bilayer graphene via interlayer spacing. Applied Physics Letters, 2008, 92, .	1.5	96
24	Topological Nodal-Net Semimetal in a Graphene Network Structure. Physical Review Letters, 2018, 120, 026402.	2.9	93
25	Photoelectron Spectra and Geometric Structures of Small Niobium Cluster Anions. Physical Review Letters, 1996, 77, 4528-4531.	2.9	80
26	Orthorhombic carbon allotrope of compressed graphite: <i>Ab initio</i> calculations. Physical Review B, 2012, 85, .	1.1	80
27	A New Carbon Allotrope with Six-Fold Helical Chains in all-sp ² Bonding Networks. Scientific Reports, 2014, 4, 4339.	1.6	77
28	Extreme Mechanics of Probing the Ultimate Strength of Nanotwinned Diamond. Physical Review Letters, 2016, 117, 116103.	2.9	75
29	Colossal Shear-Strength Enhancement of Low-Density Cubic BC ₂ N by Nanoindentation. Physical Review Letters, 2007, 98, 135505.	2.9	72
30	High-Pressure Evolution of Crystal Bonding Structures and Properties of FeOOH. Journal of Physical Chemistry Letters, 2018, 9, 2181-2185.	2.1	69
31	Rare Helium-Bearing Compound FeO_2 Stabilized at Deep-Earth Conditions. Physical Review Letters, 2018, 121, 255703.	2.9	68
32	Superconductivity in Compression-Shear Deformed Diamond. Physical Review Letters, 2020, 124, 147001.	2.9	64
33	Unraveling the structure and bonding evolution of the newly discovered iron oxide FeO_2 . Physical Review B, 2018, 98, .	2.9	61
34	Interplay of Dirac electrons and magnetism in CaMnBi ₂ and SrMnBi ₂ . Nature Communications, 2016, 7, 13833.	5.8	61
35	Indentation strength of ultraincompressible rhenium boride, carbide, and nitride from first-principles calculations. Physical Review B, 2012, 86, .	1.1	58
36	CoB_6 monolayer: A robust two-dimensional ferromagnet. Physical Review B, 2019, 99, .	2.9	58

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37	Molecular dynamics simulation of tensile elongation of carbon nanotubes: Temperature and size effects. <i>Physical Review B</i> , 2009, 79, .	1.1	55
38	Soft Bond-Deformation Paths in Superhard $\text{I}^3\text{-Boron}$. <i>Physical Review Letters</i> , 2010, 105, 215503.	2.9	55
39	Indentation Strengths of Zirconium Diboride: Intrinsic versus Extrinsic Mechanisms. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2848-2853.	2.1	54
40	Strain dependent bonding in solid C_3N_4 : High elastic moduli but low strength. <i>Physical Review B</i> , 2006, 73, .	1.1	52
41	Ultralow-Frequency Collective Compression Mode and Strong Interlayer Coupling in Multilayer Black Phosphorus. <i>Physical Review Letters</i> , 2016, 116, 087401.	2.9	51
42	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. <i>Physical Review Letters</i> , 2019, 123, 195504.	2.9	50
43	Unexpectedly low indentation strength of WB and MoB $\text{I}^3\text{-boron}$ from first principles. <i>Physical Review B</i> , 2012, 86, .	1.1	49
44	Computational prediction of body-centered cubic carbon in an all- sp^2 ring configuration. <i>Physical Review B</i> , 2015, 91, .	1.1	49
45	Fundamental constraints on the strength of transition-metal borides: The case of CrB_4 . <i>Physical Review B</i> , 2013, 87, .	1.1	46
46	Indentation-strain stiffening in tungsten nitrides: Mechanisms and implications. <i>Physical Review Materials</i> , 2020, 4, .	0.9	41
47	Structure-strength relations of distinct MoN phases from first-principles calculations. <i>Physical Review Materials</i> , 2020, 4, .	0.9	41
48	Chemically Tuning Stability and Superconductivity of $\text{P}\delta\text{-H}$ Compounds. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 935-939.	2.1	40
49	Aspect ratio dependent buckling mode transition in single-walled carbon nanotubes under compression. <i>Journal of Applied Physics</i> , 2011, 109, .	1.1	37
50	Two-dimensional ferroelectric topological insulators in functionalized atomically thin bismuth layers. <i>Physical Review B</i> , 2018, 97, .	1.1	37
51	Unraveling Convolved Structural Transitions in SnTe at High Pressure. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5352-5357.	1.5	36
52	First-principles calculation of the indentation strength of FeB_4 . <i>Physical Review B</i> , 2014, 90, .	1.1	36
53	Thermodynamic functions and pressure-temperature phase diagram of lithium alanates by <i>ab initio</i> calculations. <i>Physical Review B</i> , 2007, 76, .	1.1	34
54	Mechanism for direct conversion of graphite to diamond. <i>Physical Review B</i> , 2011, 84, .	1.1	34

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55	New carbon allotropes in $sp + sp^3$ bonding networks consisting of C_8 cubes. Physical Chemistry Chemical Physics, 2018, 20, 7962-7967.	1.3	33
56	Prediction of Above-Room-Temperature Superconductivity in Lanthanide/Actinide Extreme Superhydrides. Journal of the American Chemical Society, 2022, 144, 13394-13400.	6.6	33
57	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	1.1	31
58	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 12266-12271.	1.5	31
59	Encapsulated Silicene: A Robust Large-Gap Topological Insulator. ACS Applied Materials & Interfaces, 2015, 7, 19226-19233.	4.0	31
60	Multiferroic and Ferroic Topological Order in Ligand-Functionalized Germanene and Arsenene. Physical Review Applied, 2018, 10, .	1.5	31
61	New cubic carbon phase via graphitic sheet rumpling. Physical Review B, 2012, 85, .	1.1	30
62	Ideal tensile and shear strength of C_3N_4 . Physical Review B, 2007, 76, .	1.1	29
63	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in $sp+sp^2$ Hybrid Networks. Scientific Reports, 2016, 6, 24665.	1.6	29
64	Topological nodal line semimetal in an orthorhombic graphene network structure. Physical Review B, 2018, 97, .	1.1	29
65	Sorting transition-metal diborides: New descriptor for mechanical properties. Acta Materialia, 2021, 207, 116685.	3.8	29
66	Tetragonal Crystalline Carbon Nitrides: Theoretical Predictions. Physical Review Letters, 2001, 86, 652-655.	2.9	28
67	Tuning the magnetic and electronic properties of bilayer graphene nanoribbons on Si(001) by bias voltage. Physical Review B, 2010, 81, .	1.1	28
68	Structural and mechanical properties of partially unzipped carbon nanotubes. Physical Review B, 2011, 83, .	1.1	28
69	Tuning Magnetism of Metal Porphyrine Molecules by a Ferroelectric In_2Se_3 Monolayer. ACS Applied Materials & Interfaces, 2020, 12, 39561-39566.	4.0	27
70	Xenon iron oxides predicted as potential Xe hosts in Earth's lower mantle. Nature Communications, 2020, 11, 5227.	5.8	27
71	Diverging synthesis routes and distinct properties of cubic BC_2N at high pressure. Physical Review B, 2004, 70, .	1.1	26
72	Interlayer stacking and nature of the electronic band gap in graphitic BC_2N : First-principles pseudopotential calculations. Physical Review B, 2006, 73, .	1.1	26

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73	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
74	Unravelling the structure and strength of the highest boride of tungsten $WB_{4.2}$. Physical Review B, 2019, 100, .	1.1	25
75	Ideal strength and structural instability of aluminum at finite temperatures. Physical Review B, 2012, 86, .	1.1	24
76	Multiferroic decorated Fe_2O_3 monolayer predicted from first principles. Nanoscale, 2020, 12, 14847-14852.	2.8	24
77	Transition from band insulator to Mott insulator in one dimension: Critical behavior and phase diagram. Physical Review B, 2003, 68, .	1.1	23
78	Structural metatransition of energetically tangled crystalline phases. Physical Chemistry Chemical Physics, 2017, 19, 4560-4566.	1.3	23
79	Stability of H ₃ O 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.	3.3	23
80	Computational discovery of a new rhombohedral diamond phase. Physical Review B, 2018, 98, .	1.1	22
81	Charge carrier separation induced by intrinsic surface strain in pristine ZnO nanowires. Applied Physics Letters, 2010, 97, .	1.5	21
82	Body centered cubic carbon BC14: An all-bonded full-fledged pentadiamond. Physical Review B, 2020, 102, .	1.1	21
83	Indenter-angle-sensitive fracture modes and stress response at incipient plasticity. Physical Review B, 2009, 79, .	1.1	20
84	Kondo Signatures of a Quantum Magnetic Impurity in Topological Superconductors. Physical Review Letters, 2019, 122, 087001.	2.9	20
85	Pressure-stabilized divalent ozonide CaO ₃ and its impact on Earth's oxygen cycles. Nature Communications, 2020, 11, 4702.	5.8	20
86	Field-induced gap in the spin-1/2 antiferromagnetic Heisenberg chain: A density-matrix renormalization-group study. Physical Review B, 2002, 65, .	1.1	19
87	Highly stable and symmetric boron caged B@Co ₁₂ @B ₈₀ core-shell cluster. Applied Physics Letters, 2009, 94, 133102.	1.5	19
88	Bending manipulation induced sp ² →sp ³ bond transition in carbon nanotubes. Journal of Applied Physics, 2010, 108, .	1.1	19
89	Topological phase transition between distinct Weyl semimetal states in $MoTe_2$. Physical Review B, 2019, 100, .	1.1	19
90	Ultralow-Friction and Ultralow-Wear TiN-Ag Solid Solution Coating in Base Oil. Journal of Physical Chemistry Letters, 2020, 11, 1614-1621.	2.1	19

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91	<i>Ab initio</i> prediction of superdense tetragonal and monoclinic polymorphs of carbon. <i>Physical Review B</i> , 2016, 94, .	1.1	18
92	Topological semimetal in an sp^2 hybridized carbon network with nodal rings. <i>Physical Review B</i> , 2020, 101, .	1.1	18
93	Direct H-He chemical association in superionic FeO ₂ H ₂ He at Deep-Earth conditions. <i>National Science Review</i> , 0, .	4.6	18
94	<i>Ab initio</i> structural identification of high density cubic BC ₂ N. <i>Physical Review B</i> , 2006, 73, .	1.1	17
95	Superconductivity in Shear Strained Semiconductors. <i>Chinese Physics Letters</i> , 2021, 38, 086301.	1.3	17
96	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8437-8442.	1.5	16
97	Thermoelectric properties of rocksalt ZnO from first-principles calculations. <i>Journal of Applied Physics</i> , 2015, 118, .	1.1	16
98	Three-Dimensional Crystalline Modification of Graphene in all- sp^2 Hexagonal Lattices with or without Topological Nodal Lines. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2515-2521.	2.1	16
99	Local-Strain-Induced Charge Carrier Separation and Electronic Structure Modulation in Zigzag ZnO Nanotubes: Role of Built-In Polarization Electric Field. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2381-2385.	1.5	15
100	Robust Magnetoelectric Effect in the Decorated Graphene/In ₂ Se ₃ Heterostructure. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 3033-3039.	4.0	15
101	Pronounced Enhancement of Superconductivity in ZrN via Strain Engineering. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1985-1990.	2.1	15
102	Robust Quantum Anomalous Hall States in Monolayer and Few-Layer TiTe. <i>Nano Letters</i> , 2022, 22, 5379-5384.	4.5	15
103	Bias voltage induced n -to- p -type transition in epitaxial bilayer graphene on SiC. <i>Physical Review B</i> , 2009, 80, .	1.1	14
104	Hybrid W-shaped graphene nanoribbons: Distinct electronic and transport properties. <i>Journal of Applied Physics</i> , 2011, 110, 124312.	1.1	14
105	High-mobility anisotropic transport in few-layer β -B ₂₈ films. <i>Nanoscale</i> , 2016, 8, 20111-20117.	2.8	14
106	Stress-induced high- T_c superconductivity in solid molecular hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	14
107	NOVEL MANY-BODY EFFECTS IN PHOTOEMISSION AND INVERSE PHOTOEMISSION SPECTRA OF ULTRATHIN TRANSITION-METAL FILMS. <i>International Journal of Modern Physics B</i> , 1991, 05, 1147-1178.	1.0	13
108	Intrinsic Charge Separation and Tunable Electronic Band Gap of Armchair Graphene Nanoribbons Encapsulated in a Double-Walled Carbon Nanotube. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1328-1333.	2.1	13

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109	Influence of carbon content on the strength of cubic BC . A first-principles study. Physical Review B, 2008, 77, .	1.1	12
110	Enhancing interwall load transfer by vacancy defects in carbon nanotubes. Applied Physics Letters, 2012, 100, .	1.5	12
111	Superior magnetic and mechanical property of $MnFe$ by electron correlation and lattice anharmonicity. Physical Review B, 2015, 91, .	1.1	12
112	Structural and electronic phase transitions of ThS_2 first-principles calculations. Physical Review B, 2016, 94, .	1.1	12
113	Dual-Phase Nanocomposite $TiB_2/MoS_{1.7}B_{0.3}$: An Excellent Ultralow Friction and Ultralow Wear Self-Lubricating Material. ACS Applied Materials & Interfaces, 2021, 13, 59352-59363.	4.0	11
114	Ground-state phase diagram of a spin-12 frustrated three-leg antiferromagnetic Heisenberg ladder. Physical Review B, 2002, 66, .	1.1	10
115	Unexpected structural softening of interstitial boron solid solution WB_{3+x} . Applied Physics Letters, 2014, 105, 211901.	1.5	10
116	Ab initio study of the anharmonic lattice dynamics of iron at the $\bar{1}3\bar{1}$ phase transition. Physical Review B, 2015, 92, .	1.1	10
117	Phase stability and transition of $BaSi_2$ disilicides and digermanides. Physical Review B, 2015, 91, .	1.1	10
118	First-principles prediction of low-energy structures for AlH_3 . Physical Review B, 2009, 79, .	1.1	9
119	Anomalous strength anisotropy of $\bar{1}3\bar{1}$ -Fe ₄ N identified by first-principles calculations. Applied Physics Letters, 2009, 94, 151914.	1.5	9
120	Intrinsic low thermal conductivity in weakly ionic rocksalt structures. Physical Review B, 2015, 92, .	1.1	9
121	Topological nodal line semimetals in graphene network structures. Advances in Physics: X, 2019, 4, 1625724.	1.5	9
122	First-principles study of high-pressure phase stability and superconductivity of Bi_4I_4 . Physical Review B, 2019, 100, .	1.1	9
123	Atomistic Mechanisms for Contrasting Stress-Strain Relations of $B_{13}CN$ and $B_{13}C_2$. Journal of Physical Chemistry Letters, 2020, 11, 10454-10462.	2.1	9
124	Excitons in spatially separated electron-hole systems: A quantum Monte Carlo study. Journal of Applied Physics, 1995, 78, 7099-7102.	1.1	8
125	Probing the direct factor for superconductivity in FeSe-Based Superconductors by Raman Scattering. Physical Review B, 2019, 100, .	1.1	8
126	Extreme static compression of carbon to terapascal pressures. Carbon, 2019, 144, 161-170.	5.4	8

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127	Toughening a superstrong carbon crystal: Sequential bond-breaking mechanisms. <i>Physical Review B</i> , 2020, 102, .	1.1	8
128	Macroscale Robust Superlubricity on Metallic NbB ₂ . <i>Advanced Science</i> , 2022, 9, e2103815.	5.6	8
129	Pressure-Induced Evolution of Crystal and Electronic Structure of Ammonia Borane. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2036-2043.	2.1	7
130	Superhard metallic compound TaB_2 via crystal orientation resolved strain stiffening. <i>Physical Review B</i> , 2022, 105, .		
131	Superhard metallic compounds $\text{Sr}_5\text{Si}_3\text{N}_{12}$		

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145	Reply to "Anisotropy governs strain stiffening in nanotwinned-materials". Nature Communications, 2018, 9, 1585.	5.8	2
146	New carbon allotropes derived from nanotubes via a three-fold distortion mechanism. Physical Chemistry Chemical Physics, 2020, 22, 12489-12495.	1.3	2
147	$W \int_0^1 \frac{dx}{M(x)} \int_0^4 B(x) dx$		