Yanming

List of Publications by Year in descending order

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290 papers	26,019 citations	9234 74 h-index	7136 153 g-index
294 all docs	294 docs citations	294 times ranked	12292 citing authors

#	ARTICLE	IF	CITATIONS
1	CALYPSO: A method for crystal structure prediction. Computer Physics Communications, 2012, 183, 2063-2070.	3.0	2,085
2	Crystal structure prediction via particle-swarm optimization. Physical Review B, 2010, 82, .	1.1	1,870
3	Ionic high-pressure form of elemental boron. Nature, 2009, 457, 863-867.	13.7	803
4	Transparent dense sodium. Nature, 2009, 458, 182-185.	13.7	710
5	Ultrahard nanotwinned cubic boron nitride. Nature, 2013, 493, 385-388.	13.7	662
6	Superconductive sodalite-like clathrate calcium hydride at high pressures. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6463-6466.	3.3	630
7	The metallization and superconductivity of dense hydrogen sulfide. Journal of Chemical Physics, 2014, 140, 174712.	1.2	612
8	Nanotwinned diamond with unprecedented hardness and stability. Nature, 2014, 510, 250-253.	13.7	611
9	Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity. Physical Review Letters, 2017, 119, 107001.	2.9	591
10	Predicted Novel High-Pressure Phases of Lithium. Physical Review Letters, 2011, 106, 015503.	2.9	499
11	Superhard Monoclinic Polymorph of Carbon. Physical Review Letters, 2009, 102, 175506.	2.9	480
12	Particle-swarm structure prediction on clusters. Journal of Chemical Physics, 2012, 137, 084104.	1.2	453
13	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
14	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	23.3	427
15	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	2.9	377
16	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. Nature Chemistry, 2014, 6, 644-648.	6.6	369
17	Substitutional Alloy of Bi and Te at High Pressure. Physical Review Letters, 2011, 106, 145501.	2.9	363
18	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. Journal of Chemical Physics, 2012, 137, 224108.	1.2	275

#	ARTICLE	IF	CITATIONS
19	Pressure-stabilized superconductive yttrium hydrides. Scientific Reports, 2015, 5, 9948.	1.6	257
20	Global Structural Optimization of Tungsten Borides. Physical Review Letters, 2013, 110, 136403.	2.9	253
21	Insights into Enhanced Visible-Light Photocatalytic Hydrogen Evolution of g-C₃N₄ and Highly Reduced Graphene Oxide Composite: The Role of Oxygen. Chemistry of Materials, 2015, 27, 1612-1621.	3.2	252
22	Predicting Two-Dimensional Boronâ€“Carbon Compounds by the Global Optimization Method. Journal of the American Chemical Society, 2011, 133, 16285-16290.	6.6	242
23	Novel High Pressure Structures of Polymeric Nitrogen. Physical Review Letters, 2009, 102, 065501.	2.9	226
24	Superconducting High Pressure Phase of Germane. Physical Review Letters, 2008, 101, 107002.	2.9	224
25	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	13.7	222
26	Novel high-pressure structures of MgCO3, CaCO3 and CO2 and their role in Earth's lower mantle. Earth and Planetary Science Letters, 2008, 273, 38-47.	1.8	211
27	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. Nano Energy, 2014, 6, 219-224.	8.2	210
28	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	5.8	208
29	Two dimensional Dirac carbon allotropes from graphene. Nanoscale, 2014, 6, 1113-1118.	2.8	198
30	Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials. Reviews in Mineralogy and Geochemistry, 2010, 71, 271-298.	2.2	182
31	Superhard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BC</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>in Cubic Diamond Structure. Physical Review Letters, 2015, 114, 015502.	2.9	180
32	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	2.9	176
33	First-principles structural design of superhard materials. Journal of Chemical Physics, 2013, 138, 114101.	1.2	176
34	Tetragonal Allotrope of Group 14 Elements. Journal of the American Chemical Society, 2012, 134, 12362-12365.	6.6	170
35	High-pressure crystal structures and superconductivity of Stannane (SnH ₄). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1317-1320.	3.3	168
36	Self-assembled ultrathin nanotubes on diamond (100) surface. Nature Communications, 2014, 5, 3666.	5.8	164

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37	Origin of hardness in WB4 and its implications for ReB4, TaB4, MoB4, TcB4, and OsB4. Applied Physics Letters, 2008, 93, .	1.5	154
38	B₃₈: an all-boron fullerene analogue. Nanoscale, 2014, 6, 11692-11696.	2.8	153
39	Novel Structures and Superconductivity of Silane under Pressure. Physical Review Letters, 2009, 102, 087005.	2.9	146
40	Crystal Structures and Exotic Behavior of Magnesium under Pressure. Journal of Physical Chemistry C, 2010, 114, 21745-21749.	1.5	146
41	Crystalline LiN₅ Predicted from First-Principles as a Possible High-Energy Material. Journal of Physical Chemistry Letters, 2015, 6, 2363-2366.	2.1	145
42	Structural Modifications and Mechanical Properties of Molybdenum Borides from First Principles. Journal of Physical Chemistry C, 2010, 114, 6722-6725.	1.5	142
43	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	1.4	138
44	Perspective: Crystal structure prediction at high pressures. Journal of Chemical Physics, 2014, 140, 040901.	1.2	135
45	High-pressure structures of lithium, potassium, and rubidium predicted by anab initioevolutionary algorithm. Physical Review B, 2008, 78, .	1.1	132
46	Superconductivity at â^¼100ÂK in dense SiH ₄ (H ₂) ₂ predicted by first principles. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15708-15711.	3.3	132
47	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	2.9	132
48	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. Physical Review Letters, 2017, 119, 115503.	2.9	129
49	Phase stability and mechanical properties of tungsten borides from first principles calculations. Physical Chemistry Chemical Physics, 2010, 12, 13158.	1.3	126
50	Dissociation products and structures of solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:math>at strong compression. Physical Review B, 2016, 93, .	1.1	119
51	Metastable 1Tâ€²-phase group VIB transition metal dichalcogenide crystals. Nature Materials, 2021, 20, 1113-1120.	13.3	119
52	Predicted Lithiumâ€“Boron Compounds under High Pressure. Journal of the American Chemical Society, 2012, 134, 18599-18605.	6.6	113
53	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. Physical Review B, 2008, 77, .	1.1	112
54	Spiral chain O ₄ form of dense oxygen. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 751-753.	3.3	111

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55	Structural Evolution of Carbon Dioxide under High Pressure. Journal of the American Chemical Society, 2013, 135, 14167-14171.	6.6	111
56	Superconductivity in Pristine <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>2</mml:mn><mml:msub><mml:mrow><mml:mi>H</mml:mi></mml:mrow><mml:mrow><mml:mi></mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> at Ultrahigh Pressure. Physical Review Letters, 2018, 120, 037002.	2.9	109
57	A novel low compressible and superhard carbon nitride: Body-centered tetragonal CN2. Physical Chemistry Chemical Physics, 2012, 14, 13081.	1.3	108
58	Enhanced thermoelectric performance of PbTe within the orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>P</mml:mi><mml:mi>n</mml:mi><mml:mi>m</mml:mi><mml:mi>a</mml:mi></mml:mrow></mml:math> Physical Review B, 2007, 76, .	1.1	107
59	Structure of the metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î¶</mml:mi></mml:math>-phase of oxygen and isosymmetric nature of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Îµ</mml:mi><mml:mtext>â”</mml:mtext><mml:mi>Î¶</mml:mi></mml:mrow></mml:math> phase. Physical Review B, 2007, 76, .	1.1	107
60	Anomalous Stress Response of Ultrahard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WB</mml:mi></mml:mrow><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2015, 115, 185502.	2.9	107
61	Superconducting high-pressure phases of disilane. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9969-9973.	3.3	102
62	Dissociation of methane under high pressure. Journal of Chemical Physics, 2010, 133, 144508.	1.2	101
63	Gold as a 6p-Element in Dense Lithium Aurides. Journal of the American Chemical Society, 2016, 138, 4046-4052.	6.6	101
64	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
65	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	0.7	93
66	Superconductivity in high-pressure SiH 4. Europhysics Letters, 2007, 78, 37003.	0.7	89
67	Ordering of Hydrogen Bonds in High-Pressure Low-TemperatureH2O. Physical Review Letters, 2005, 94, 025502.	2.9	86
68	Exotic behavior and crystal structures of calcium under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 7646-7651.	3.3	86
69	Exploring Hardness and the Distorted sp² Hybridization of Bâ€“B Bonds in WB₃. Chemistry of Materials, 2014, 26, 5297-5302.	3.2	80
70	Ab initiostudy revealing a layered structure in hydrogen-rich KH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>under high pressure. Physical Review B, 2012, 86, .	1.1	79
71	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
72	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. Journal of Physical Chemistry C, 2012, 116, 9221-9226.	1.5	78

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73	First-principles study of elastic and vibrational properties of the Heusler-type alloys<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub>	1.1	77
74	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. Faraday Discussions, 2018, 211, 31-43.	1.6	76
75	First-principles studies of structural and electronic properties of hexagonalBC5. Physical Review B, 2006, 73, .	1.1	75
76	Metallic Icosahedron Phase of Sodium at Terapascal Pressures. Physical Review Letters, 2015, 114, 125501.	2.9	75
77	Two-dimensional boronâ€“nitrogenâ€“carbon monolayers with tunable direct band gaps. Nanoscale, 2015, 7, 12023-12029.	2.8	74
78	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	2.8	72
79	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	1.6	71
80	Ultrastrong Boron Frameworks in ZrB₁₂: A Highway for Electron Conducting. Advanced Materials, 2017, 29, 1604003.	11.1	71
81	Computer-Assisted Inverse Design of Inorganic Electrides. Physical Review X, 2017, 7, .	2.8	70
82	Room-temperature structures of solid hydrogen at high pressures. Journal of Chemical Physics, 2012, 137, 074501.	1.2	69
83	Insight into the role of Li₂S₂ in Liâ€“S batteries: a first-principles study. Journal of Materials Chemistry A, 2015, 3, 8865-8869.	5.2	68
84	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. Chemistry of Materials, 2016, 28, 1746-1755.	3.2	68
85	A Protocol to Fabricate Nanostructured New Phase: B31-Type MnS Synthesized under High Pressure. Journal of the American Chemical Society, 2015, 137, 10297-10303.	6.6	67
86	Superhard and superconducting structures of BC5. Journal of Applied Physics, 2010, 108, .	1.1	66
87	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. Solid State Communications, 2007, 141, 610-614.	0.9	65
88	Metallic and superconducting gallane under high pressure. Physical Review B, 2011, 84, .	1.1	65
89	Novel High Pressure Structures and Superconductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ca</mml:mi><mml:msub><mml:mi>Li</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2010, 104, 177005.	2.9	64
90	Superconductivity in Compression-Shear Deformed Diamond. Physical Review Letters, 2020, 124, 147001.	2.9	64

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91	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. Physical Review B, 2013, 88, .	1.1	63
92	Electronic and dynamical properties of NiAl studied from first principles. Intermetallics, 2011, 19, 1959-1967.	1.8	62
93	Exotic high pressure behavior of light alkali metals, lithium and sodium. European Physical Journal B, 2011, 81, 1-14.	0.6	62
94	Superhard semiconductingC3N2compounds predicted via first-principles calculations. Physical Review B, 2008, 78, .	1.1	60
95	Superhard and superconductive polymorphs of diamond-like BC3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 771-774.	0.9	59
96	Proton or Deuteron Transfer in Phase IV of Solid Hydrogen and Deuterium. Physical Review Letters, 2013, 110, 025903.	2.9	59
97	Ultra-incompressible phases of tungsten dinitride predicted from first principles. Physical Review B, 2009, 79, .	1.1	58
98	Hydrogenâ€rich superconductors at high pressures. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1330.	6.2	57
99	Electron-phonon coupling ofÎ±â^'Gaboron. Physical Review B, 2004, 70, .	1.1	54
100	Electronic structure, phase stability, and hardness of the osmium borides, carbides, nitrides, and oxides: First-principles calculations. Journal of Physics and Chemistry of Solids, 2008, 69, 2096-2102.	1.9	54
101	Rhombohedral superhard structure of BC2N. Journal of Applied Physics, 2009, 105, 053514.	1.1	54
102	Enhanced Vickers hardness by quasi-3D boron network in MoB2. RSC Advances, 2013, 3, 18317.	1.7	53
103	A Stable, Magnetic, and Metallic Li3O4Compound as a Discharge Product in a Liâ€"Air Battery. Journal of Physical Chemistry Letters, 2014, 5, 2516-2521.	2.1	52
104	Metallization and superconductivity of BeH2 under high pressure. Journal of Chemical Physics, 2014, 140, 124707.	1.2	50
105	Stable xenon nitride at high pressures. Physical Review B, 2015, 92, .	1.1	50
106	A two-dimensional TiB₄monolayer exhibits planar octacoordinate Ti. Nanoscale, 2017, 9, 17983-17990.	2.8	50
107	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. Physical Review Letters, 2019, 123, 195504.	2.9	50
108	High-Pressure Structural Transitions of Sc₂O₃ by X-ray Diffraction, Raman Spectra, and Ab Initio Calculations. Inorganic Chemistry, 2009, 48, 8251-8256.	1.9	49

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109	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	1.5	49
110	Superconductivity in lithium under high pressure investigated with density functional and Eliashberg theory. Physical Review B, 2009, 79, .	1.1	48
111	Polymorphism and Formation Mechanism of Nanobipods in Manganese Sulfide Nanocrystals Induced by Temperature or Pressure. Journal of Physical Chemistry C, 2012, 116, 3292-3297.	1.5	48
112	Twofold Coordinated Ground-State and Eightfold High-Pressure Phases of Heavy Transition Metal Nitrides MN₂ (M = Os, Ir, Ru, and Rh). Inorganic Chemistry, 2009, 48, 9904-9909.	1.9	47
113	Predicting new superhard phases. Journal of Superhard Materials, 2010, 32, 192-204.	0.5	46
114	Determination of Structures, Stabilities, and Electronic Properties for Bimetallic Cesium-Doped Gold Clusters: A Density Functional Theory Study. Journal of Physical Chemistry A, 2011, 115, 9273-9281.	1.1	46
115	Pressure-Induced Formation of Noble Metal Hydrides. Journal of Physical Chemistry C, 2012, 116, 1995-2000.	1.5	46
116	Phonon instabilities in rocksalt AgCl and AgBr under pressure studied within density functional theory. Physical Review B, 2006, 74, .	1.1	45
117	High-pressure and high-temperature phase transitions in FeTiO3 and a new dense FeTi3O7 structure. American Mineralogist, 2012, 97, 568-572.	0.9	45
118	Absence of superconductivity in the high-pressure polymorph of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 79, .	1.1	43
119	Stabilization of 9/10-Fold Structure in Bismuth Selenide at High Pressures. Journal of Physical Chemistry C, 2013, 117, 10045-10050.	1.5	43
120	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
121	Determinations of the high-pressure crystal structures of Sb₂Te₃. Journal of Physics Condensed Matter, 2012, 24, 475403.	0.7	42
122	Prediction of Silicon-Based Layered Structures for Optoelectronic Applications. Journal of the American Chemical Society, 2014, 136, 15992-15997.	6.6	42
123	Mercury under Pressure acts as a Transition Metal: Calculated from First Principles. Angewandte Chemie - International Edition, 2015, 54, 9280-9283.	7.2	42
124	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	3.0	42
125	First-Principles Prediction on the High-Pressure Structures of Transition Metal Diborides (TMB₂, TM = Sc, Ti, Y, Zr). Inorganic Chemistry, 2010, 49, 6859-6864.	1.9	41
126	Carbon-in-Al₄C₃ Nanowire Superstructures for Field Emitters. ACS Nano, 2011, 5, 932-941.	7.3	41

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127	Lattice dynamics and elastic properties of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:math>electron system: CeN. Physical Review B, 2011, 84, .	1.1	41
128	Unexpected Trend in Stability of Xeâ€“F Compounds under Pressure Driven by Xeâ€“Xe Covalent Bonds. Journal of Physical Chemistry Letters, 2016, 7, 4562-4567.	2.1	41
129	High-temperature superconductivity on the verge of a structural instability in lanthanum superhydride. Nature Communications, 2021, 12, 6863.	5.8	40
130	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	1.2	40
131	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. Physical Review B, 2007, 75, .	1.1	39
132	Structural morphologies of high-pressure polymorphs of strontium hydrides. Physical Chemistry Chemical Physics, 2015, 17, 19379-19385.	1.3	39
133	Superhard polymorphs of diamond-like. Solid State Communications, 2011, 151, 716-719.	0.9	38
134	Synthesis and high-pressure transformation of metastable wurtzite-structured CuGaS2 nanocrystals. Nanoscale, 2012, 4, 7443.	2.8	38
135	Tetragonal high-pressure phase of ZnO predicted from first principles. Physical Review B, 2009, 79, .	1.1	37
136	B ₂ CO: A potential superhard material in the B-C-O system. Europhysics Letters, 2011, 95, 66006.	0.7	37
137	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. Matter and Radiation at Extremes, 2020, 5, .	1.5	37
138	ScandiumâEDoped AlN 1D Hexagonal Nanoprisms: A Class of RoomâETemperature Ferromagnetic Materials. Angewandte Chemie - International Edition, 2010, 49, 173-176.	7.2	36
139	High Thermoelectric Performance of Ge/Si Coreâ^'Shell Nanowires: First-Principles Prediction. Journal of Physical Chemistry C, 2010, 114, 9096-9100.	1.5	36
140	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. Journal of Physical Chemistry C, 2013, 117, 5352-5357.	1.5	36
141	Structure Prediction of Atoms Adsorbed on Two-Dimensional Layer Materials: Method and Applications. Journal of Physical Chemistry C, 2015, 119, 20111-20118.	1.5	36
142	Ab initiostudies of solid bromine under high pressure. Physical Review B, 2007, 76, .	1.1	35
143	Stabilization of ammonia-rich hydrate inside icy planets. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9003-9008.	3.3	35
144	Electron-phonon coupling in high-pressure Nb. Physical Review B, 2004, 69, .	1.1	34

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145	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	1.6	34
146	CaCl2-type high-pressure phase of magnesium hydride predicted byab initiophonon calculations. Physical Review B, 2007, 75, .	1.1	33
147	HgTe: A potential thermoelectric material in the cinnabar phase. Journal of Chemical Physics, 2008, 128, 194713.	1.2	33
148	Unexpected Roomâ€Temperature Ferromagnetism in Nanostructured Bi₂Te₃. Angewandte Chemie - International Edition, 2014, 53, 729-733.	7.2	33
149	Prediction of Above-Room-Temperature Superconductivity in Lanthanide/Actinide Extreme Superhydrides. Journal of the American Chemical Society, 2022, 144, 13394-13400.	6.6	33
150	Prediction of a new layered phase of nitrogen from first-principles simulations. Journal of Physics Condensed Matter, 2007, 19, 425226.	0.7	32
151	Nanocrystalline tungsten hydrides at high pressures. Physical Review B, 2013, 87, .	1.1	32
152	Nb-H system at high pressures and temperatures. Physical Review B, 2017, 95, .	1.1	32
153	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 12266-12271.	1.5	31
154	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	0.7	31
155	First-principles study of the mechanisms for the pressure-induced phase transitions in zinc-blende CuBr and CuI. Physical Review B, 2004, 69, .	1.1	30
156	Atomistic Design of High Thermoelectricity on Si/Ge Superlattice Nanowires. Journal of Physical Chemistry C, 2011, 115, 20696-20702.	1.5	30
157	Pressure-Induced Reversible Phase Transformation in Nanostructured Bi₂Te₃ with Reduced Transition Pressure. Journal of Physical Chemistry C, 2015, 119, 3843-3848.	1.5	30
158	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	3.0	30
159	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. APL Materials, 2015, 3, .	2.2	29
160	Design of ternary alkaline-earth metal Sn(<scp>ii</scp>) oxides with potential good p-type conductivity. Journal of Materials Chemistry C, 2016, 4, 4592-4599.	2.7	29
161	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	4.0	29
162	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied usingab initiocalculations. Physical Review B, 2007, 75, .	1.1	28

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163	Exploring High-Pressure Lithium Beryllium Hydrides: A New Chemical Perspective. Journal of Physical Chemistry C, 2013, 117, 13879-13886.	1.5	28
164	Nitrogen Backbone Oligomers. Scientific Reports, 2015, 5, 13239.	1.6	28
165	Stabilization of H3+ in the high pressure crystalline structure of HnCl (n = 2â€“7). Chemical Science, 2015, 6, 522-526.	3.7	28
166	Superconductivity in simple elemental solidsâ€”a computational study of boron-doped diamond and high pressure phases of Li and Si. Journal of Physics Condensed Matter, 2005, 17, S911-S920.	0.7	27
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