Yanming

List of Publications by Citations

287 papers	20,535 citations	67 h-index	136 g-index
294 ext. papers	23,542 ext. citations	6.4 avg, IF	6.96 L-index

#	Paper	IF	Citations
287	CALYPSO: A method for crystal structure prediction. *Computer Physics Communications*, **2012**, 183, 2063-2070	4.2	1464
286	Crystal structure prediction via particle-swarm optimization. *Physical Review B*, **2010**, 82,	3.3	1446
285	Ionic high-pressure form of elemental boron. *Nature*, **2009**, 457, 863-7	50.4	680
284	Transparent dense sodium. *Nature*, **2009**, 458, 182-5	50.4	584
283	Ultrahard nanotwinned cubic boron nitride. *Nature*, **2013**, 493, 385-8	50.4	519
282	The metallization and superconductivity of dense hydrogen sulfide. *Journal of Chemical Physics*, **2014**, 140, 174712	3.9	481
281	Superconductive sodalite-like clathrate calcium hydride at high pressures. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 6463-6	11.5	449
280	Nanotwinned diamond with unprecedented hardness and stability. *Nature*, **2014**, 510, 250-3	50.4	440
279	Superhard monoclinic polymorph of carbon. *Physical Review Letters*, **2009**, 102, 175506	7.4	434
278	Predicted novel high-pressure phases of lithium. *Physical Review Letters*, **2011**, 106, 015503	7.4	429
277	Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity. *Physical Review Letters*, **2017**, 119, 107001	7.4	352
276	Particle-swarm structure prediction on clusters. *Journal of Chemical Physics*, **2012**, 137, 084104	3.9	340
275	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
274	Substitutional alloy of Bi and Te at high pressure. *Physical Review Letters*, **2011**, 106, 145501	7.4	318
273	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. *Nature Chemistry*, **2014**, 6, 644-8	17.6	314
272	High-pressure hydrogen sulfide from first principles: a strongly anharmonic phonon-mediated superconductor. *Physical Review Letters*, **2015**, 114, 157004	7.4	299
271	Materials discovery at high pressures. *Nature Reviews Materials*, **2017**, 2,	73.3	266

270	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. *Journal of Chemical Physics*, **2012**, 137, 224108	3.9	223
269	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	9.6	219
268	Global structural optimization of tungsten borides. *Physical Review Letters*, **2013**, 110, 136403	7.4	216
267	Predicting two-dimensional boron-carbon compounds by the global optimization method. *Journal of the American Chemical Society*, **2011**, 133, 16285-90	16.4	209
266	Superconducting high pressure phase of germane. *Physical Review Letters*, **2008**, 101, 107002	7.4	204
265	High pressure partially ionic phase of water ice. *Nature Communications*, **2011**, 2, 563	17.4	201
264	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	5.3	187
263	Pressure-stabilized superconductive yttrium hydrides. *Scientific Reports*, **2015**, 5, 9948	4.9	184
262	Novel high pressure structures of polymeric nitrogen. *Physical Review Letters*, **2009**, 102, 065501	7.4	181
261	Oxygen-doped boron nitride nanosheets with excellent performance in hydrogen storage. *Nano Energy*, **2014**, 6, 219-224	17.1	170
260	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. *Nature*, **2016**, 532, 81-4	50.4	165
259	High-pressure crystal structures and superconductivity of Stannane (SnH4). *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 1317-20	11.5	153
258	First-principles structural design of superhard materials. *Journal of Chemical Physics*, **2013**, 138, 114101	3.9	151
257	Two dimensional Dirac carbon allotropes from graphene. *Nanoscale*, **2014**, 6, 1113-8	7.7	147
256	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147
255	Tetragonal allotrope of group 14 elements. *Journal of the American Chemical Society*, **2012**, 134, 12362-5	16.4	146
254	Evolutionary Crystal Structure Prediction as a Method for the Discovery of Minerals and Materials. *Reviews in Mineralogy and Geochemistry*, **2010**, 71, 271-298	7.1	143
253	Origin of hardness in WB4 and its implications for ReB4, TaB4, MoB4, TcB4, and OsB4. *Applied Physics Letters*, **2008**, 93, 101905	3.4	140

252	Cagelike diamondoid nitrogen at high pressures. *Physical Review Letters*, **2012**, 109, 175502	7.4	139
251	Novel structures and superconductivity of silane under pressure. *Physical Review Letters*, **2009**, 102, 087005	7.4	137
250	Self-assembled ultrathin nanotubes on diamond (100) surface. *Nature Communications*, **2014**, 5, 3666	17.4	133
249	B38: an all-boron fullerene analogue. *Nanoscale*, **2014**, 6, 11692-6	7.7	127
248	Structural Modifications and Mechanical Properties of Molybdenum Borides from First Principles. *Journal of Physical Chemistry C*, **2010**, 114, 6722-6725	3.8	125
247	Superconductivity at approximately 100 K in dense SiH4(H2)2 predicted by first principles. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 15708-11	11.5	121
246	Crystal Structures and Exotic Behavior of Magnesium under Pressure. *Journal of Physical Chemistry C*, **2010**, 114, 21745-21749	3.8	121
245	Perspective: crystal structure prediction at high pressures. *Journal of Chemical Physics*, **2014**, 140, 040901	3.9	116
244	Extraordinary Indentation Strain Stiffening Produces Superhard Tungsten Nitrides. *Physical Review Letters*, **2017**, 119, 115503	7.4	108
243	High-pressure structures of lithium, potassium, and rubidium predicted by an ab initio evolutionary algorithm. *Physical Review B*, **2008**, 78,	3.3	108
242	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. *Physical Review Letters*, **2016**, 116, 057002	7.4	104
241	Spiral chain O form of dense oxygen. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 751-3	11.5	104
240	Phase stability and mechanical properties of tungsten borides from first principles calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 13158-65	3.6	104
239	CALYPSO structure prediction method and its wide application. *Computational Materials Science*, **2016**, 112, 406-415	3.2	102
238	Structural evolution of carbon dioxide under high pressure. *Journal of the American Chemical Society*, **2013**, 135, 14167-71	16.4	101
237	Enhanced thermoelectric performance of PbTe within the orthorhombic Pnma phase. *Physical Review B*, **2007**, 76,	3.3	99
236	Crystalline LiN5 Predicted from First-Principles as a Possible High-Energy Material. *Journal of Physical Chemistry Letters*, **2015**, 6, 2363-6	6.4	98
235	Dissociation products and structures of solid H2S at strong compression. *Physical Review B*, **2016**, 93,	3.3	96

234	Structure of the metallic □phase of oxygen and isosymmetric nature of the □phase transition: Ab initio simulations. *Physical Review B*, **2007**, 76,	3.3	96
233	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Physical Review B*, **2008**, 77,	3.3	95
232	Predicted lithium-boron compounds under high pressure. *Journal of the American Chemical Society*, **2012**, 134, 18599-605	16.4	93
231	A novel low compressible and superhard carbon nitride: body-centered tetragonal CN2. *Physical Chemistry Chemical Physics*, **2012**, 14, 13081-7	3.6	91
230	Superconducting high-pressure phases of disilane. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9969-73	11.5	91
229	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. *Physical Review B*, **2005**, 72,	3.3	89
228	Dissociation of methane under high pressure. *Journal of Chemical Physics*, **2010**, 133, 144508	3.9	86
227	Anomalous Stress Response of Ultrahard WB_{n} Compounds. *Physical Review Letters*, **2015**, 115, 185502	7.4	85
226	Superconductivity in high-pressure SiH 4. *Europhysics Letters*, **2007**, 78, 37003	1.6	82
225	Exotic behavior and crystal structures of calcium under pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 7646-51	11.5	74
224	Ordering of hydrogen bonds in high-pressure low-temperature H2O. *Physical Review Letters*, **2005**, 94, 025502	7.4	72
223	Gold as a 6p-Element in Dense Lithium Aurides. *Journal of the American Chemical Society*, **2016**, 138, 4046-52	13.4	70
222	First-principles studies of structural and electronic properties of hexagonal BC5. *Physical Review B*, **2006**, 73,	3.3	70
221	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. *Journal of Physical Chemistry C*, **2012**, 116, 9221-9226	3.8	67
220	Density functional study of elastic and vibrational properties of the Heusler-type alloys Fe2VAl and Fe2VGa. *Physical Review B*, **2009**, 80,	3.3	64
219	Room-temperature structures of solid hydrogen at high pressures. *Journal of Chemical Physics*, **2012**, 137, 074501	3.9	64
218	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. *Nanoscale*, **2015**, 7, 12023-9	7.7	63
217	Materials discovery via CALYPSO methodology. *Journal of Physics Condensed Matter*, **2015**, 27, 203203	1.8	63

216	Ab initio study revealing a layered structure in hydrogen-rich KH6 under high pressure. *Physical Review B*, **2012**, 86,	3.3	63
215	Superconductivity in Pristine 2H_{a}-MoS_{2} at Ultrahigh Pressure. *Physical Review Letters*, **2018**, 120, 037002	7.4	62
214	Superhard and superconducting structures of BC5. *Journal of Applied Physics*, **2010**, 108, 023507	2.5	60
213	Stabilization of fullerene-like boron cages by transition metal encapsulation. *Nanoscale*, **2015**, 7, 10482-9	7.7	59
212	Exploring Hardness and the Distorted sp2 Hybridization of BB Bonds in WB3. *Chemistry of Materials*, **2014**, 26, 5297-5302	9.6	59
211	Metallic and superconducting gallane under high pressure. *Physical Review B*, **2011**, 84,	3.3	58
210	Insight into the role of Li2S2 in LiS batteries: a first-principles study. *Journal of Materials Chemistry A*, **2015**, 3, 8865-8869	13	57
209	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. *Chemistry of Materials*, **2016**, 28, 1746-1755	9.6	57
208	Proton or deuteron transfer in phase IV of solid hydrogen and deuterium. *Physical Review Letters*, **2013**, 110, 025903	7.4	57
207	Metallic icosahedron phase of sodium at terapascal pressures. *Physical Review Letters*, **2015**, 114, 125501	7.4	56
206	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
205	Exotic high pressure behavior of light alkali metals, lithium and sodium. *European Physical Journal B* , **2011**, 81, 1-14	1.2	56
204	A Protocol to Fabricate Nanostructured New Phase: B31-Type MnS Synthesized under High Pressure. *Journal of the American Chemical Society*, **2015**, 137, 10297-303	16.4	55
203	Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Physical Review B*, **2009**, 79,	3.3	55
202	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. *Solid State Communications*, **2007**, 141, 610-614	1.6	55
201	Novel high pressure structures and superconductivity of CaLi2. *Physical Review Letters*, **2010**, 104, 177005	7.4	54
200	Superhard and superconductive polymorphs of diamond-like BC3. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2011**, 375, 771-774	2.3	53
199	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. *Physical Review B*, **2013**, 88,	3.3	52

198	Rhombohedral superhard structure of BC2N. *Journal of Applied Physics*, **2009**, 105, 053514	2.5	52
197	Computer-Assisted Inverse Design of Inorganic Electrides. *Physical Review X*, **2017**, 7,	9.1	51
196	Electron-phonon coupling of Ga boron. *Physical Review B*, **2004**, 70,	3.3	51
195	Ultrastrong Boron Frameworks in ZrB : A Highway for Electron Conducting. *Advanced Materials*, **2017**, 29, 1604003	24	50
194	Superhard semiconducting C3N2 compounds predicted via first-principles calculations. *Physical Review B*, **2008**, 78,	3.3	50
193	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	3.9	50
192	A Stable, Magnetic, and Metallic Li3O4 Compound as a Discharge Product in a Li-Air Battery. *Journal of Physical Chemistry Letters*, **2014**, 5, 2516-21	6.4	48
191	Twofold coordinated ground-state and eightfold high-pressure phases of heavy transition metal nitrides MN(2) (M = Os, Ir, Ru, and Rh). *Inorganic Chemistry*, **2009**, 48, 9904-9	5.1	46
190	Electronic and dynamical properties of NiAl studied from first principles. *Intermetallics*, **2011**, 19, 1959-1967	3.9	45
189	Enhanced Vickers hardness by quasi-3D boron network in MoB2. *RSC Advances*, **2013**, 3, 18317	3.7	42
188	Pressure-Induced Formation of Noble Metal Hydrides. *Journal of Physical Chemistry C*, **2012**, 116, 1995-2000	3.8	42
187	Superconductivity in lithium under high pressure investigated with density functional and Eliashberg theory. *Physical Review B*, **2009**, 79,	3.3	42
186	Phonon instabilities in rocksalt AgCl and AgBr under pressure studied within density functional theory. *Physical Review B*, **2006**, 74,	3.3	42
185	Hydrogen-rich superconductors at high pressures. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1330	7.9	41
184	Accelerating CALYPSO structure prediction by data-driven learning of a potential energy surface. *Faraday Discussions*, **2018**, 211, 31-43	3.6	40
183	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, 9273-81	2.8	40
182	High-pressure structural transitions of Sc2O3 by X-ray diffraction, Raman spectra, and ab initio calculations. *Inorganic Chemistry*, **2009**, 48, 8251-6	5.1	40
181	Predicting new superhard phases. *Journal of Superhard Materials*, **2010**, 32, 192-204	0.9	40

180	Metallization and superconductivity of BeH2 under high pressure. *Journal of Chemical Physics*, **2014** , 140, 124707	3.9	39
179	Stable xenon nitride at high pressures. *Physical Review B*, **2015**, 92,	3.3	39
178	Polymorphism and Formation Mechanism of Nanobipods in Manganese Sulfide Nanocrystals Induced by Temperature or Pressure. *Journal of Physical Chemistry C*, **2012**, 116, 3292-3297	3.8	39
177	Absence of superconductivity in the high-pressure polymorph of MgB2. *Physical Review B*, **2009**, 79,	3.3	39
176	First-principles study of the lattice dynamics, thermodynamic properties and electron-phonon coupling of YB6. *Physical Review B*, **2007**, 76,	3.3	39
175	Stabilization of 9/10-Fold Structure in Bismuth Selenide at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 10045-10050	3.8	38
174	Carbon-in-Al4C3 nanowire superstructures for field emitters. *ACS Nano*, **2011**, 5, 932-41	16.7	38
173	Two-Dimensional C4N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. *Journal of Physical Chemistry C*, **2017**, 121, 2669-2674	3.8	37
172	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. *Physical Review B*, **2007**, 75,	3.3	37
171	Prediction of silicon-based layered structures for optoelectronic applications. *Journal of the American Chemical Society*, **2014**, 136, 15992-7	16.4	36
170	High-pressure and high-temperature phase transitions in FeTiO3 and a new dense FeTi3O7 structure. *American Mineralogist*, **2012**, 97, 568-572	2.9	36
169	Metastable 1TRphase group VIB transition metal dichalcogenide crystals. *Nature Materials*, **2021**, 20, 1113-1120	27	36
168	Unraveling Convoluted Structural Transitions in SnTe at High Pressure. *Journal of Physical Chemistry C*, **2013**, 117, 5352-5357	3.8	35
167	Mercury under Pressure acts as a Transition Metal: Calculated from First Principles. *Angewandte Chemie - International Edition*, **2015**, 54, 9280-3	16.4	34
166	High Thermoelectric Performance of Ge/Si Core–Shell Nanowires: First-Principles Prediction. *Journal of Physical Chemistry C*, **2010**, 114, 9096-9100	3.8	34
165	B 2 CO: A potential superhard material in the B-C-O system. *Europhysics Letters*, **2011**, 95, 66006	1.6	34
164	Superhard polymorphs of diamond-like BC7. *Solid State Communications*, **2011**, 151, 716-719	1.6	34
163	Scandium-doped AlN 1D hexagonal nanoprisms: a class of room-temperature ferromagnetic materials. *Angewandte Chemie - International Edition*, **2010**, 49, 173-6	16.4	34

162	Superconductivity in Compression-Shear Deformed Diamond. *Physical Review Letters*, **2020**, 124, 147001	7.4	33
161	Unexpected Trend in Stability of Xe-F Compounds under Pressure Driven by Xe-Xe Covalent Bonds. *Journal of Physical Chemistry Letters*, **2016**, 7, 4562-4567	6.4	33
160	Determinations of the high-pressure crystal structures of Sb2Te3. *Journal of Physics Condensed Matter*, **2012**, 24, 475403	1.8	33
159	Tetragonal high-pressure phase of ZnO predicted from first principles. *Physical Review B*, **2009**, 79,	3.3	33
158	CaCl2-type high-pressure phase of magnesium hydride predicted by ab initio phonon calculations. *Physical Review B*, **2007**, 75,	3.3	33
157	Synthesis and high-pressure transformation of metastable wurtzite-structured CuGaS2 nanocrystals. *Nanoscale*, **2012**, 4, 7443-7	7.7	32
156	Ab initio studies of solid bromine under high pressure. *Physical Review B*, **2007**, 76,	3.3	32
155	Unexpected room-temperature ferromagnetism in nanostructured Bi2Te3. *Angewandte Chemie - International Edition*, **2014**, 53, 729-33	16.4	31
154	Electron-phonon coupling in high-pressure Nb. *Physical Review B*, **2004**, 69,	3.3	31
153	First-principles study of the mechanisms for the pressure-induced phase transitions in zinc-blende CuBr and CuI. *Physical Review B*, **2004**, 69,	3.3	30
152	Structural morphologies of high-pressure polymorphs of strontium hydrides. *Physical Chemistry Chemical Physics*, **2015**, 17, 19379-85	3.6	29
151	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, **2016**, 200, 87-95	4.2	29
150	Lattice dynamics and elastic properties of the 4f electron system: CeN. *Physical Review B*, **2011**, 84,	3.3	29
149	First-principles prediction on the high-pressure structures of transition metal diborides (TMB2, TM = Sc, Ti, Y, Zr). *Inorganic Chemistry*, **2010**, 49, 6859-64	5.1	29
148	HgTe: a potential thermoelectric material in the cinnabar phase. *Journal of Chemical Physics*, **2008**, 128, 194713	3.9	29
147	A two-dimensional TiB monolayer exhibits planar octacoordinate Ti. *Nanoscale*, **2017**, 9, 17983-17990	7.7	28
146	Structure Prediction of Atoms Adsorbed on Two-Dimensional Layer Materials: Method and Applications. *Journal of Physical Chemistry C*, **2015**, 119, 20111-20118	3.8	28
145	Nanocrystalline tungsten hydrides at high pressures. *Physical Review B*, **2013**, 87,	3.3	28

144	Nb-H system at high pressures and temperatures. *Physical Review B*, **2017**, 95,	3.3	27
143	Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity. *Physical Review Letters*, **2019**, 123, 195504	7.4	27
142	Nitrogen Backbone Oligomers. *Scientific Reports*, **2015**, 5, 13239	4.9	27
141	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. *APL Materials*, **2015**, 3, 011102	5.7	27
140	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	11.5	26
139	Stable Lithium Argon compounds under high pressure. *Scientific Reports*, **2015**, 5, 16675	4.9	26
138	High-pressure phase transitions of solid HF, HCl, and HBr: An ab initio evolutionary study. *Physical Review B*, **2010**, 82,	3.3	26
137	Electronic and phonon instabilities in face-centered-cubic alkali metals under pressure studied using ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	26
136	Superconductivity in simple elemental solids□ computational study of boron-doped diamond and high pressure phases of Li and Si. *Journal of Physics Condensed Matter*, **2005**, 17, S911-S920	1.8	26
135	Pressure-induced phonon instabilities in copper chloride. *Physical Review B*, **2003**, 67,	3.3	26
134	Stabilization of H in the high pressure crystalline structure of H Cl (= 2-7). *Chemical Science*, **2015**, 6, 522-526	9.4	25
133	Pressure-Induced Reversible Phase Transformation in Nanostructured Bi2Te3 with Reduced Transition Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 3843-3848	3.8	25
132	Atomistic Design of High Thermoelectricity on Si/Ge Superlattice Nanowires. *Journal of Physical Chemistry C*, **2011**, 115, 20696-20702	3.8	25
131	Pressure-induced enhancement of electron-phonon coupling in superconducting CaC6 from first principles. *Physical Review B*, **2006**, 74,	3.3	25
130	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. *Journal of Physical Chemistry C* , **2013**, 117, 12266-12271	3.8	24
129	Origin of the High Thermoelectric Performance in Si Nanowires: A First-Principle Study. *Journal of Physical Chemistry C*, **2009**, 113, 14001-14005	3.8	23
128	Prediction of a new layered phase of nitrogen from first-principles simulations. *Journal of Physics Condensed Matter*, **2007**, 19, 425226	1.8	23
127	Pressure-induced phase transformations in the Ba8Si46 clathrate. *Physical Review B*, **2006**, 74,	3.3	23

126	Design of ternary alkaline-earth metal Sn(II) oxides with potential good p-type conductivity. *Journal of Materials Chemistry C*, **2016**, 4, 4592-4599	7.1	23
125	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896	9.5	22
124	Exploring High-Pressure Lithium Beryllium Hydrides: A New Chemical Perspective. *Journal of Physical Chemistry C*, **2013**, 117, 13879-13886	3.8	22
123	Superconducting high-pressure phase of cesium iodide. *Physical Review B*, **2009**, 79,	3.3	22
122	X-ray diffraction data-assisted structure searches. *Computer Physics Communications*, **2017**, 213, 40-45	4.2	21
121	Origin of bcc to fcc phase transition under pressure in alkali metals. *New Journal of Physics*, **2008**, 10, 063022	2.9	21
120	Structural metatransition of energetically tangled crystalline phases. *Physical Chemistry Chemical Physics*, **2017**, 19, 4560-4566	3.6	20
119	The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr2FeMoO6: A theoretical study. *Solid State Communications*, **2014**, 177, 57-60	1.6	20
118	Orientationally disordered H2 in the high-pressure van der Waals compound SiH4(H2)2. *Physical Review B*, **2010**, 82,	3.3	20
117	Effect of nonhydrostatic pressure on superconductivity of monatomic iodine: An ab initio study. *Physical Review B*, **2009**, 79,	3.3	20
116	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. *Chemical Science*, **2014**, 5, 3936-3940	9.4	19
115	Ultra-incompressible superconducting phase of OsC predicted by phonon calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 1880-1884	2.3	18
114	Novel phases in ammonia-water mixtures under pressure. *Journal of Chemical Physics*, **2018**, 149, 234501	3.9	18
113	Construction of crystal structure prototype database: methods and applications. *Journal of Physics Condensed Matter*, **2017**, 29, 165901	1.8	17
112	Superhard-driven search of the covalent network in the B3NO system. *RSC Advances*, **2015**, 5, 35882-35887	3.7	17
111	One-Dimensional Al4O4C Ceramics: A New Type of Blue Light Emitter. *Scientific Reports*, **2013**, 3,	4.9	17
110	High-pressure phase transitions in NiAs-type compounds from first-principles calculations. *Physical Review B*, **2010**, 81,	3.3	17
109	Design of Superhard Ternary Compounds under High Pressure: SiC2N4 and Si2CN4. *Journal of Physical Chemistry C*, **2010**, 114, 8609-8613	3.8	17

108	Crystal structure and physical properties of OsN: First-principle calculations. *Solid State Communications*, **2010**, 150, 759-762	1.6	17
107	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. *Matter and Radiation at Extremes*, **2020**, 5, 068101	4.7	17
106	Carbon coated face-centered cubic Ru-C nanoalloys. *Nanoscale*, **2014**, 6, 10370-6	7.7	16
105	Structural and mechanical properties of platinum carbide. *Inorganic Chemistry*, **2014**, 53, 5797-802	5.1	16
104	Sn(II)-Containing Phosphates as Optoelectronic Materials. *Chemistry of Materials*, **2017**, 29, 2459-2465	9.6	16
103	Modulated structure and molecular dissociation of solid chlorine at high pressures. *Journal of Chemical Physics*, **2012**, 137, 064502	3.9	16
102	Order-disorder phase transition and dissociation of hydrogen sulfide under high pressure: ab initio molecular dynamics study. *Journal of Chemical Physics*, **2010**, 132, 164506	3.9	16
101	Prediction study of the axial compressibility, anisotropy and dynamic properties for single crystal Ti2GeC. *Journal of Alloys and Compounds*, **2010**, 506, 22-26	5.7	16
100	Structural phase transformations of Mg(3)N(2) at high pressure: experimental and theoretical studies. *Inorganic Chemistry*, **2009**, 48, 9737-41	5.1	16
99	High pressure structures of "111" type iron-based superconductors predicted from first-principles. *Physical Chemistry Chemical Physics*, **2012**, 14, 15029-35	3.6	15
98	Crystal structures, stability, electronic and elastic properties of 4d and 5d transition metal monoborides: First-principles calculations. *Journal of Alloys and Compounds*, **2012**, 538, 115-124	5.7	15
97	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. *Journal of Physical Chemistry C*, **2013**, 117, 8437-8442	3.8	15
96	Raman evidence of a new high-pressure phase in calcium hydride. *Journal of Physics Condensed Matter*, **2007**, 19, 226205	1.8	15
95	First-principle optimal local pseudopotentials construction via optimized effective potential method. *Journal of Chemical Physics*, **2016**, 144, 134108	3.9	15
94	Effects of manganese doping on the structure evolution of small-sized boron clusters. *Journal of Physics Condensed Matter*, **2017**, 29, 265401	1.8	14
93	Investigations on structural determination of semi-transition-metal borides. *Physical Chemistry Chemical Physics*, **2017**, 19, 31592-31598	3.6	14
92	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. *Scientific Reports*, **2015**, 5, 13039	4.9	14
91	Pressure induced phase transitions in TiH2. *Journal of Applied Physics*, **2013**, 113, 103512	2.5	14

90	Superhard phases of B2O: An isoelectronic compound of diamond. *Diamond and Related Materials*, **2011**, 20, 501-504	3.5	14
89	The effects of pressure on the electronic, transport and dynamical properties of AuX2(X = Al, Ga and In). *Journal of Physics Condensed Matter*, **2007**, 19, 425224	1.8	14
88	Structural evolution of FeH4 under high pressure. *RSC Advances*, **2017**, 7, 12570-12575	3.7	13
87	Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. *Journal of Chemical Physics*, **2012**, 137, 184502	3.9	13
86	The pressure-induced phase transition in SnO: a first-principles study. *Journal of Physics Condensed Matter*, **2007**, 19, 425230	1.8	13
85	Chemical bonding, electron-phonon coupling, and structural transformations in high-pressure phases of Si. *Journal of Physical Chemistry B*, **2006**, 110, 3721-6	3.4	13
84	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 24996-25002	3.8	12
83	High-pressure structures and metallization of sodium chloride. *Europhysics Letters*, **2012**, 100, 26005	1.6	12
82	Superconductivity of MgB2 under ultrahigh pressure: A first-principles study. *Physical Review B*, **2009**, 80,	3.3	12
81	Phase-transition mechanism of h-BN -ω-BN from first principles. *Solid State Communications*, **2009**, 149, 843-846	1.6	12
80	First-principles studies of phonon instabilities in AgI under high pressure. *Journal of Physics Condensed Matter*, **2008**, 20, 195218	1.8	12
79	Ab initiolattice dynamics evidence for the broken-symmetry phase of solid hydrogen. *Journal of Physics Condensed Matter*, **2006**, 18, 9917-9927	1.8	12
78	Phase transition in a classical two-dimensional electron system. *Physical Review B*, **2003**, 68,	3.3	12
77	Silicon Framework-Based Lithium Silicides at High Pressures. *ACS Applied Materials & Interfaces* , **2016**, 8, 16761-7	9.5	11
76	High-pressure phase transition of cesium chloride and cesium bromide. *Physical Chemistry Chemical Physics*, **2014**, 16, 17924-9	3.6	11
75	Phase transition of cadmium fluoride under high pressure. *Solid State Communications*, **2011**, 151, 1899-1902	1.8	11
74	Superconductivity and lattice instability in face-centered cubic lanthanum under high pressure. *Journal of Physics Condensed Matter*, **2007**, 19, 425234	1.8	11
73	A first-principles study of electron–phonon coupling in electron-doped LiH. *Journal of Physics Condensed Matter*, **2007**, 19, 425218	1.8	11

72	Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principles. *Applied Surface Science*, **2017**, 393, 422-427	6.7	10
71	Anomalous Melting Behavior of Solid Hydrogen at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 11873-11877	3.8	10
70	Tian et al. reply. *Nature*, **2013**, 502, E2-3	50.4	10
69	Pressure-induced elemental dissociation in zinc chalcogenides. *New Journal of Physics*, **2010**, 12, 043058	2.9	10
68	Crystal structures of under high pressure. *Solid State Communications*, **2011**, 151, 388-391	1.6	10
67	Superconductivity in high-pressure solids. *Journal of Physics Condensed Matter*, **2007**, 19, 425208	1.8	10
66	Magnetism in Na-filled Fe-based skutterudites. *Scientific Reports*, **2015**, 5, 10782	4.9	9
65	Two-dimensional silicon monolayers generated on c-BN(111) substrate. *Physical Chemistry Chemical Physics*, **2015**, 17, 15694-700	3.6	9
64	First-principles study of the magnetic, structural and electronic properties of LiFeAs. *Journal of Physics Condensed Matter*, **2010**, 22, 046006	1.8	9
63	The crystal structure and superconducting properties of monatomic bromine. *Journal of Physics Condensed Matter*, **2010**, 22, 015702	1.8	9
62	Pressure-induced amorphization in mayenite (12CaO□7Al2O3). *Journal of Chemical Physics*, **2011**, 135, 094506	3.9	9
61	Peierls transition in sodium under high pressure: a first-principles study. *Journal of Physics Condensed Matter*, **2009**, 21, 025508	1.8	9
60	Valence band x-ray emission spectra of compressed germanium. *Physical Review Letters*, **2006**, 96, 137402	7.4	9
59	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. *Physical Review B*, **2016**, 94,	3.3	9
58	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
57	Gluing together metallic and covalent layers to form Ru2C under ambient conditions. *Physical Chemistry Chemical Physics*, **2015**, 17, 9730-6	3.6	8
56	First-principles study of phase transitions in antiferromagnetic □(, Co and Ni). *Solid State Communications*, **2011**, 151, 1475-1478	1.6	8
55	Novel superhard polymorphs of Be3N2 predicted by first-principles. *Computational Materials Science*, **2010**, 49, S76-S79	3.2	8

54	First-principles studies of phonon softening in rocksalt AgF under pressure. *Journal of Physics Condensed Matter*, **2007**, 19, 425217	1.8	8
53	Pressure-induced magnetic transition in metallic nickel hydrides by ab initio pseudopotential plane-wave calculations. *Physical Review B*, **2006**, 74,	3.3	8
52	A symmetry-orientated divide-and-conquer method for crystal structure prediction.. *Journal of Chemical Physics*, **2022**, 156, 014105	3.9	8
51	Prediction of Host-Guest Na-Fe Intermetallics at High Pressures. *Inorganic Chemistry*, **2016**, 55, 7026-32	5.1	8
50	The diverse electronic properties of C4N3monolayer under biaxial compressive strain: a theoretical study. *Journal Physics D: Applied Physics*, **2016**, 49, 295301	3	7
49	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. *Journal of Physical Chemistry C*, **2014**, 118, 11902-11905	3.8	7
48	High pressure–low temperature phase diagram of barium: Simplicity versus complexity. *Applied Physics Letters*, **2015**, 107, 221908	3.4	7
47	Inter- and Intralayer Compression of Germanane. *Journal of Physical Chemistry C*, **2014**, 118, 28196-28201	3.8	7
46	Dynamic nano-pulling effect of the boron-functionalized graphene monovacancy for molecule dissociation. *Journal Physics D: Applied Physics*, **2013**, 46, 385302	3	7
45	Raman Scattering Study of AlN Nanowires under High Pressure. *Journal of Physical Chemistry C*, **2010**, 114, 8241-8244	3.8	7
44	Ab initio study of vacancies in cubic BN under pressure. *Solid State Communications*, **2007**, 143, 532-536	1.6	7
43	Phase boundary between the fractional quantum Hall liquid and the Wigner crystal at low filling factors and low temperatures: A path integral Monte Carlo study. *Physical Review B*, **2005**, 72,	3.3	7
42	Computational discovery and characterization of new BO phases. *Physical Chemistry Chemical Physics*, **2019**, 21, 2499-2506	3.6	6
41	Globally stable structures of LixZn (x = 1-4) compounds at high pressures. *Physical Chemistry Chemical Physics*, **2016**, 18, 4437-43	3.6	6
40	Orientation dependence of elastic constants and electronic properties of rhenium nitrides first-principle calculations. *Journal of Materials Science*, **2013**, 48, 4284-4296	4.3	6
39	Room-temperature ferromagnetism of 2H-SiC–Al2O3 solid solution nanowires and the physical origin. *Nanoscale*, **2015**, 7, 4912-9	7.7	6
38	The broken-symmetry phase of solid hydrogen: evidence from infrared and Raman active vibrons. *Journal of Physics Condensed Matter*, **2007**, 19, 425237	1.8	6
37	High-temperature superconductivity on the verge of a structural instability in lanthanum superhydride. *Nature Communications*, **2021**, 12, 6863	17.4	6

36	Xenon iron oxides predicted as potential Xe hosts in Earth's lower mantle. *Nature Communications*, **2020**, 11, 5227	17.4	6
35	O(NlogN) scaling method to evaluate the ion-electron potential of crystalline solids. *Journal of Chemical Physics*, **2016**, 145, 184110	3.9	6
34	Calculated high-pressure structural properties, lattice dynamics and quasi particle band structures of perovskite fluorides KZnF3, CsCaF3 and BaLiF3. *Journal of Physics Condensed Matter*, **2016**, 28, 315403	1.8	5
33	Elastic anisotropy and phonon focusing in NiAl: Atomic study. *Intermetallics*, **2013**, 42, 156-164	3.5	5
32	Lattice instability and martensitic transformation in LaAg predicted from first-principles theory. *Journal of Physics Condensed Matter*, **2012**, 24, 075402	1.8	5
31	Catenation of carbon in LaC2 predicted under high pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 14286-91	3.6	5
30	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. *RSC Advances*, **2015**, 5, 104426-104432	3.7	4
29	Size-dependent phase transition of graphite to superhard graphite under high pressure at room temperature. *Journal of Applied Physics*, **2012**, 112, 103707	2.5	4
28	Phase transition and optical properties of CaCl2under high pressure byab initiopseudopotential plane-wave calculations. *Journal of Physics Condensed Matter*, **2007**, 19, 425225	1.8	4
27	First-principles study of high-pressure phase stability and superconductivity of Bi4I4. *Physical Review B*, **2019**, 100,	3.3	4
26	Ground-State Crystal Structure of Strontium Peroxide Predicted from First Principles. *Inorganic Chemistry*, **2017**, 56, 7545-7549	5.1	3
25	Exploring the high pressure behavior of 2D and quasi-3D boron layers in MoB2. *RSC Advances*, **2014**, 4, 52878-52882	3.7	3
24	Pressure-induced isostructural phase transition in CaB4. *RSC Advances*, **2014**, 4, 42523-42529	3.7	3
23	Acoustic waves and phonon focus in Li crystal: the first principle study. *European Physical Journal B*, **2014**, 87, 1	1.2	3
22	Spectroscopic and Computational Characterizations of Alkaline-Earth- and Heavy-Metal-Exchanged Natrolites. *ChemPlusChem*, **2014**, 79, 1096-1102	2.8	3
21	High-pressure polymorphs of Li(2)BeH(4) predicted by first-principles calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 385405	1.8	3
20	Electronic and optical properties of orthorhombic and hexagonal phases of CsMgH3: First-principles calculations. *Physica B: Condensed Matter*, **2009**, 404, 1061-1069	2.8	3
19	First-principles supercell studies of the substitutional carbon in c-BN. *Diamond and Related Materials*, **2008**, 17, 2025-2028	3.5	3

18	Materials by design at high pressures.. *Chemical Science*, **2022**, 13, 329-344	9.4	3
17	Pressure-stabilized divalent ozonide CaO and its impact on Earth's oxygen cycles. *Nature Communications*, **2020**, 11, 4702	17.4	3
16	Theoretical realization of half-metallicity in two-dimensional monolayered molybdenum dinitride by Mo vacancy tuning. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2016**, 380, 2669-2673	2.2	3
15	A database assisted protein structure prediction method via a swarm intelligence algorithm. *RSC Advances*, **2017**, 7, 39869-39876	3.7	2
14	First-principles study on mechanical and magnetic properties of the perovskite and post-perovskite polymorphs of pure end-member FeSiO3 at the core–mantle boundary. *High Pressure Research*, **2010**, 30, 292-300	1.6	2
13	Ab initio simulation of core-hole effects on the X-ray absorption near edge structure of GaP. *Physica B: Condensed Matter*, **2009**, 404, 1643-1647	2.8	2
12	Structural and dynamical properties of H2S under high pressure:ab initiomolecular dynamics studies. *Journal of Physics Condensed Matter*, **2007**, 19, 425232	1.8	2
11	Experimental clathrate superhydrides EuH6 and EuH9 at extreme pressure conditions. *Physical Review Research*, **2021**, 3,	3.9	2
10	Magnetism and thermodynamic properties of a spin-1/2 ferrimagnetic diamond XY chain in magnetic fields at finite temperatures. *Journal of the Korean Physical Society*, **2013**, 62, 104-115	0.6	1
9	Comment on "Pressure-dependent metallic and superconducting phases in a germanium artificial metal". *Physical Review Letters*, **2010**, 104, 139701; author reply 139702	7.4	1
8	Structural Investigation of Solid Methane at High Pressure. *Chinese Physics Letters*, **2010**, 27, 066101	1.8	1
7	The influence of defects on the transport properties of AgSbPb18Te20prepared at high pressure and high temperature. *Journal of Physics Condensed Matter*, **2007**, 19, 425219	1.8	1
6	Low-Pressure Electrochemical Synthesis of Complex High-Pressure Superconducting Superhydrides.. *Physical Review Letters*, **2022**, 128, 186001	7.4	0
5	Evolutionary Crystal Structure Prediction and Novel High-Pressure Phases. *NATO Science for Peace and Security Series B: Physics and Biophysics*, **2010**, 293-323	0.2	
4	Influence of impurity hydrogen on the structure and properties of bulk Li and pressure effects **2006**, 49, 740-747		
3	Pressure effects on the absorption spectra of Na doped in solid Ar **2004**, 47, 550		
2	Temperature Effects on the Absorption Spectra of Li in Solid H2 Under High Pressure: A Path Integral Monte Carlo Study. *Journal of Low Temperature Physics*, **2001**, 124, 587-598	1.3	
1	Properties and order-disorder competition of spin-1/2 XY model in the ferrimagnetic diamond chain. *Wuli Xuebao/Acta Physica Sinica*, **2012**, 61, 187502	0.6	