Hanyu Liu

List of Publications by Year in Descending Order

176 papers	6,750 citations	41 h-index	78 g-index
197 ext. papers	8,447 ext. citations	5.7 avg, IF	6.23 L-index

#	Paper	IF	Citations
176	A symmetry-orientated divide-and-conquer method for crystal structure prediction.. *Journal of Chemical Physics*, **2022**, 156, 014105	3.9	8
175	Phase transition and electronic properties of barium fluoride at high pressure. *Solid State Communications*, **2022**, 342, 114597	1.6	0
174	Structure search of two-dimensional systems using CALYPSO methodology. *Frontiers of Physics*, **2022**, 17, 1	3.7	1
173	High-Temperature Superconducting Phase in Clathrate Calcium Hydride CaH_{6} up to 215□K at a Pressure of 172□GPa.. *Physical Review Letters*, **2022**, 128, 167001	7.4	9
172	Low-Pressure Electrochemical Synthesis of Complex High-Pressure Superconducting Superhydrides.. *Physical Review Letters*, **2022**, 128, 186001	7.4	0
171	Prediction of stable Cu structure and phase transition mechanism at ultra-high pressure: A comprehensive properties characterization by DFT calculation. *Physica B: Condensed Matter*, **2021**, 413538	2.8	
170	Experimental clathrate superhydrides EuH6 and EuH9 at extreme pressure conditions. *Physical Review Research*, **2021**, 3,	3.9	2
169	Superconductivity of H3S doped with light elements. *Physical Review Research*, **2021**, 3,	3.9	4
168	Prediction of high-Tc superconductivity in ternary lanthanum borohydrides. *Physical Review B*, **2021**, 104,	3.3	13
167	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. *Chemistry - A European Journal*, **2021**, 27, 17420-17427	4.8	0
166	Stable Structures and Superconductivity in a Y-Si System under High Pressure. *Journal of Physical Chemistry Letters*, **2021**, 12, 10388-10393	6.4	3
165	Quantum and Classical Proton Diffusion in Superconducting Clathrate Hydrides. *Physical Review Letters*, **2021**, 126, 117002	7.4	6
164	Potassium-activated anionic copper and covalent Cu-Cu bonding in compressed K-Cu compounds. *Journal of Chemical Physics*, **2021**, 154, 134708	3.9	1
163	Superconductivity in metal intercalated graphite-like boron-carbon-nitrogen. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2021**, 402, 127348	2.3	0
162	Superconductive Sodium Carbides with Pentagon Carbon at High Pressures. *Journal of Physical Chemistry Letters*, **2021**, 12, 5850-5856	6.4	2
161	Retainable Superconductivity and Structural Transition in 1T-TaSe Under High Pressure. *Inorganic Chemistry*, **2021**, 60, 11385-11393	5.1	1
160	Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. *Physical Chemistry Chemical Physics*, **2021**, 23, 21544-21553	3.6	1

159	Machine learning metadynamics simulation of reconstructive phase transition. *Physical Review B*, **2021**, 103,	3.3	6
158	Predicted Stable Structures of the Li-Ag System at High Pressures. *Journal of Physical Chemistry Letters*, **2021**, 12, 1671-1675	6.4	4
157	Superconductive hydrogen-rich compounds under high pressure. *Applied Physics A: Materials Science and Processing*, **2021**, 127, 1	2.6	0
156	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
155	Exploring the structures and properties of nickel silicides at the pressures of the Earth's core. *Physical Chemistry Chemical Physics*, **2021**, 23, 14671-14677	3.6	4
154	Pressure-induced superconductivity and structure phase transition in Pt2HgSe3. *Npj Quantum Materials*, **2021**, 6,	5	2
153	Structure and superconductivity in compressed Li-Si-H compounds: Density functional theory calculations. *Physical Review B*, **2020**, 102,	3.3	6
152	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
151	Predicted CsSi compound: a promising material for photovoltaic applications. *Physical Chemistry Chemical Physics*, **2020**, 22, 11578-11582	3.6	3
150	Computational prediction of a +4 oxidation state in Au via compressed AuO compound. *Journal of Physics Condensed Matter*, **2020**, 32, 015402	1.8	0
149	An automated predictor for identifying transition states in solids. *Npj Computational Materials*, **2020**, 6,	10.9	5
148	Chemically Tuning Stability and Superconductivity of P-H Compounds. *Journal of Physical Chemistry Letters*, **2020**, 11, 935-939	6.4	21
147	Superconducting thorium hydrides under high pressure. *Solid State Communications*, **2020**, 309, 113820	1.6	3
146	Bi and Sn Co-doping Enhanced Thermoelectric Properties of CuSbS Materials with Excellent Thermal Stability. *ACS Applied Materials & Interfaces*, **2020**, 12, 8271-8279	9.5	14
145	Pressure-Tuned Core/Shell Configuration Transition of Shell Thickness-Dependent CdSe/CdS Nanocrystals. *Journal of Physical Chemistry Letters*, **2020**, 11, 920-926	6.4	6
144	Route to high-Tc superconductivity via CH4-intercalated H3S hydride perovskites. *Physical Review B* , **2020**, 101,	3.3	45
143	Pressure-induced decomposition of binary lanthanum intermetallic compounds. *Physical Review B*, **2020**, 101,	3.3	4
142	Structural characteristics and elasticities of coesite and coesite-II at high pressure. *New Journal of Physics*, **2020**, 22, 093044	2.9	

141	Theoretical design of two-dimensional carbon nitrides. *Nanotechnology*, **2020**, 31, 495707	3.4	4
140	Oxysulfide Li2BeSO: A potential new material for solid electrolyte predicted from first principles. *Journal of Alloys and Compounds*, **2020**, 818, 152844	5.7	1
139	Carbon-boron clathrates as a new class of sp-bonded framework materials. *Science Advances*, **2020**, 6, eaay8361	14.3	20
138	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. *Chemistry of Materials*, **2020**, 32, 459-467	9.6	18
137	A General Route to Prepare Low-Ruthenium-Content Bimetallic Electrocatalysts for pH-Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. *Angewandte Chemie*, **2020**, 132, 1735-1743	3.6	26
136	A General Route to Prepare Low-Ruthenium-Content Bimetallic Electrocatalysts for pH-Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. *Angewandte Chemie - International Edition*, **2020**, 59, 1718-1726	16.4	250
135	A new intermediate phase in compressed nitinol. *Journal of Alloys and Compounds*, **2020**, 817, 153234	5.7	1
134	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. *Matter and Radiation at Extremes*, **2020**, 5, 068101	4.7	17
133	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. *Journal of Physical Chemistry Letters*, **2020**, 11, 8710-8720	6.4	18
132	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. *Physical Review Letters*, **2019**, 123, 097001	7.4	125
131	Decomposition and Recombination of Binary Interalkali NaK at High Pressures. *Journal of Physical Chemistry Letters*, **2019**, 10, 3006-3012	6.4	7
130	Synthesis and stability of tantalum hydride at high pressures. *Physical Review B*, **2019**, 99,	3.3	13
129	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. *Journal of Physical Chemistry Letters*, **2019**, 10, 2761-2766	6.4	17
128	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. *Physical Review B*, **2019**, 99,	3.3	7
127	Hard BN Clathrate Superconductors. *Journal of Physical Chemistry Letters*, **2019**, 10, 2554-2560	6.4	9
126	Effect of the Inherent Structure of Rh Nanocrystals on the Hydriding Behavior under Pressure. *Journal of Physical Chemistry Letters*, **2019**, 10, 774-779	6.4	3
125	Identifying the Ground-State NP Sheet through a Global Structure Search in Two-Dimensional Space and Its Promising High-Efficiency Photovoltaic Properties **2019**, 1, 375-382		20
124	Theoretical investigation of the valence states in Au via the Au-F compounds under high pressure. *Physical Chemistry Chemical Physics*, **2019**, 21, 17621-17627	3.6	5

123	Synergistic effects of reduced graphene oxide with freeze drying tuned interfacial structure on performance of transparent and flexible supercapacitors. *Journal of Colloid and Interface Science*, **2019**, 554, 650-657	9.3	4
122	High-pressure modulated structures in beryllium chalcogenides. *Physical Review B*, **2019**, 100,	3.3	2
121	First-principles study of crystal structures and superconductivity of ternary YSH6 and LaSH6 at high pressures. *Physical Review B*, **2019**, 100,	3.3	16
120	A high-entropy metal oxide as chemical anchor of polysulfide for lithium-sulfur batteries. *Energy Storage Materials*, **2019**, 23, 678-683	19.4	81
119	Superconducting TaH5 at high pressure. *New Journal of Physics*, **2019**, 21, 123009	2.9	4
118	First-principles molecular dynamics simulations of single nitrogen bond structures in a N2H2 system under pressure. *Solid State Communications*, **2019**, 290, 27-30	1.6	1
117	Novel high-pressure structure and superconductivity of titanium trisulfide. *Computational Materials Science*, **2019**, 158, 192-196	3.2	2
116	Route to high-energy density polymeric nitrogen t-N via He-N compounds. *Nature Communications*, **2018**, 9, 722	17.4	95
115	First principles study of LiAlO: new dense monoclinic phase under high pressure. *Journal of Physics Condensed Matter*, **2018**, 30, 115401	1.8	2
114	A combined experimental and theoretical investigation of donor and acceptor interface in efficient aqueous-processed polymer/nanocrystal hybrid solar cells. *Science China Chemistry*, **2018**, 61, 437-443	7.9	6
113	Synthesis of Xenon and Iron-Nickel Intermetallic Compounds at Earth's Core Thermodynamic Conditions. *Physical Review Letters*, **2018**, 120, 096001	7.4	28
112	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of NaGe. *Inorganic Chemistry*, **2018**, 57, 2002-2012	5.1	7
111	Crystal Structures and Electronic Properties of Xe□l Compounds at High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 2941-2950	3.8	4
110	Shock compression behavior of a mixture of cubic and hexagonal boron nitride. *Journal of Applied Physics*, **2018**, 123, 175903	2.5	5
109	High-pressure phase transitions of nitinol NiTi to a semiconductor with an unusual topological structure. *Physical Review B*, **2018**, 97,	3.3	5
108	Theoretical research on novel orthorhombic tungsten dinitride from first principles calculations.. *RSC Advances*, **2018**, 8, 9272-9276	3.7	3
107	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. *Journal of Physical Chemistry C*, **2018**, 122, 19370-19378	3.8	27
106	Unexpected Semimetallic BiS at High Pressure and High Temperature. *Journal of Physical Chemistry Letters*, **2018**, 9, 5785-5791	6.4	10

105	Semiconducting cubic titanium nitride in the Th3P4 structure. *Physical Review Materials*, **2018**, 2,	3.2	17
104	Synthesis of new nickel hydrides at high pressure. *Physical Review Materials*, **2018**, 2,	3.2	10
103	Synthesis and Stability of Lanthanum Superhydrides. *Angewandte Chemie - International Edition*, **2018**, 57, 688-692	16.4	134
102	Synthesis and Stability of Lanthanum Superhydrides. *Angewandte Chemie*, **2018**, 130, 696-700	3.6	10
101	Phase transition and superconductivity in ReS, ReSe and ReTe. *Physical Chemistry Chemical Physics*, **2018**, 20, 29472-29479	3.6	11
100	Carbon network evolution from dimers to sheets in superconducting ytrrium dicarbide under pressure. *Communications Chemistry*, **2018**, 1,	6.3	8
99	Prediction of Stable Iron Nitrides at Ambient and High Pressures with Progressive Formation of New Polynitrogen Species. *Chemistry of Materials*, **2018**, 30, 8476-8485	9.6	33
98	Rare Helium-Bearing Compound FeO_{2}He Stabilized at Deep-Earth Conditions. *Physical Review Letters*, **2018**, 121, 255703	7.4	38
97	Predicting the structure and stability of titanium oxide electrides. *Npj Computational Materials*, **2018**, 4,	10.9	16
96	Dynamics and superconductivity in compressed lanthanum superhydride. *Physical Review B*, **2018**, 98,	3.3	53
95	Crystal Structures and Properties of Iron Hydrides at High Pressure. *Journal of Physical Chemistry C*, **2018**, 122, 24262-24269	3.8	15
94	Pressure-induced structural modulations in coesite. *Physical Review B*, **2018**, 98,	3.3	2
93	Janus CoN/Co cocatalyst in porous N-doped carbon: toward enhanced catalytic activity for hydrogen evolution. *Catalysis Science and Technology*, **2018**, 8, 3695-3703	5.5	31
92	Reply to Datchi et al.: Recovered phase CO2-V at low temperature and a newly predicted 3D-extended CO2 phase. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E658-E659	11.5	1
91	Two-Dimensional C4N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. *Journal of Physical Chemistry C*, **2017**, 121, 2669-2674	3.8	37
90	Toward ultrafast lithium ion capacitors: A novel atomic layer deposition seeded preparation of Li4Ti5O12/graphene anode. *Nano Energy*, **2017**, 36, 46-57	17.1	115
89	Potential high- superconducting lanthanum and yttrium hydrides at high pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 6990-6995	11.5	387
88	Crystal Structures of CaBN at High Pressures. *Inorganic Chemistry*, **2017**, 56, 7449-7453	5.1	1

87	Nb-H system at high pressures and temperatures. *Physical Review B*, **2017**, 95,	3.3	27
86	Divergent synthesis routes and superconductivity of ternary hydride MgSiH6 at high pressure. *Physical Review B*, **2017**, 96,	3.3	32
85	Electron-phonon coupling mechanisms for hydrogen-rich metals at high pressure. *Physical Review B* , **2017**, 96,	3.3	35
84	Novel boron channel-based structure of boron carbide at high pressures. *Journal of Physics Condensed Matter*, **2017**, 29, 455401	1.8	1
83	Melting and High P-T Transitions of Hydrogen up to 300 GPa. *Physical Review Letters*, **2017**, 119, 075302	7.4	33
82	BC8 Silicon (Si-III) is a Narrow-Gap Semiconductor. *Physical Review Letters*, **2017**, 118, 146601	7.4	35
81	Single-bonded allotrope of nitrogen predicted at high pressure. *Physical Review B*, **2017**, 96,	3.3	27
80	Pressure-induced polyamorphism in a main-group metallic glass. *Physical Review B*, **2016**, 94,	3.3	11
79	Metadynamics investigations of the AlN/GaN superlattice. *Europhysics Letters*, **2016**, 114, 46002	1.6	1
78	Synthesis of Bulk BC8 Silicon Allotrope by Direct Transformation and Reduced-Pressure Chemical Pathways. *Inorganic Chemistry*, **2016**, 55, 8943-50	5.1	17
77	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. *Scientific Reports*, **2016**, 6, 18918	4.9	5
76	Crystal structures and dynamical properties of dense CO2. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 11110-11115	11.5	23
75	Dissociation products and structures of solid H2S at strong compression. *Physical Review B*, **2016**, 93,	3.3	96
74	Superconductivity in dense carbon-based materials. *Physical Review B*, **2016**, 93,	3.3	18
73	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. *Physical Review Letters*, **2016**, 116, 057002	7.4	104
72	Different evolutionary pathways from B4 to B1 phase in AlN and InN: metadynamics investigations. *Journal of Physics Condensed Matter*, **2016**, 28, 205403	1.8	13
71	Stable Calcium Nitrides at Ambient and High Pressures. *Inorganic Chemistry*, **2016**, 55, 7550-5	5.1	51
70	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. *Journal of Physical Chemistry Letters*, **2016**, 7, 4898-4904	6.4	8

69	Structure and Electronic Properties of FeSH Compound under High Pressure. *Inorganic Chemistry*, **2016**, 55, 11434-11439	5.1	35
68	Crystal Structure and Superconductivity of PH3 at High Pressures. *Journal of Physical Chemistry C*, **2016**, 120, 3458-3461	3.8	59
67	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. *Nature*, **2016**, 532, 81-4	50.4	165
66	Predicted lithium–iron compounds under high pressure. *RSC Advances*, **2016**, 6, 66721-66728	3.7	4
65	Prediction of Host-Guest Na-Fe Intermetallics at High Pressures. *Inorganic Chemistry*, **2016**, 55, 7026-32	5.1	8
64	High-pressure crystal structures of TaAs from first-principles calculations. *Solid State Communications*, **2016**, 240, 37-40	1.6	6
63	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiBC11 and Li2B2C10. *RSC Advances*, **2016**, 6, 52695-52699	3.7	2
62	High pressure polyhydrides of molybdenum: A first-principles study. *Solid State Communications*, **2016**, 239, 14-19	1.6	13
61	A New Allotrope of Nitrogen as High-Energy Density Material. *Journal of Physical Chemistry A*, **2016**, 120, 2920-5	2.8	49
60	Crystal structures and superconductivity of technetium hydrides under pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 28791-28796	3.6	10
59	Dense Hydrocarbon Structures at Megabar Pressures. *Journal of Physical Chemistry Letters*, **2016**, 7, 4218-4222	6.4	22
58	A new high-pressure polymeric nitrogen phase in potassium azide. *RSC Advances*, **2015**, 5, 11825-11830	3.7	16
57	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. *Nanoscale*, **2015**, 7, 12023-9	7.7	63
56	Predicted two-dimensional electrides: Lithium–carbon monolayer sheet. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2015**, 379, 2511-2514	2.3	10
55	Compressed sodalite-like MgH6 as a potential high-temperature superconductor. *RSC Advances*, **2015**, 5, 59292-59296	3.7	104
54	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. *Scientific Reports*, **2015**, 5, 11381	4.9	18
53	High-pressure hydrogen sulfide from first principles: a strongly anharmonic phonon-mediated superconductor. *Physical Review Letters*, **2015**, 114, 157004	7.4	299
52	Crystal Structures and Chemical Bonding of Magnesium Carbide at High Pressure. *Journal of Physical Chemistry C*, **2015**, 119, 23168-23174	3.8	16

51	Ambient-Pressure Polymerization of Carbon Anions in the High-Pressure Phase Mg2C. *Inorganic Chemistry*, **2015**, 54, 10761-5	5.1	4
50	Polymerization of Nitrogen in Ammonium Azide at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 25268-25272	3.8	14
49	Pressure-Induced Structures and Properties in Indium Hydrides. *Inorganic Chemistry*, **2015**, 54, 9924-8	5.1	23
48	Unraveling Stable Vanadium Tetraboride and Triboride by First-Principles Computations. *Journal of Physical Chemistry C*, **2015**, 119, 21649-21657	3.8	25
47	Structures and stability of novel transition-metal (M=Co,Rh,CoandIr) borides. *Physical Review B*, **2015**, 92,	3.3	7
46	Prediction of the XeHe binary phase diagram at high pressures. *Chemical Physics Letters*, **2015**, 640, 115-118	2.5	7
45	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. *Scientific Reports*, **2015**, 5, 15433	4.9	56
44	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. *Scientific Reports*, **2015**, 5, 13039	4.9	14
43	High-Energy Density and Superhard Nitrogen-Rich B-N Compounds. *Physical Review Letters*, **2015**, 115, 105502	7.4	106
42	The electrical conductivity of Al2O3 under shock-compression. *Scientific Reports*, **2015**, 5, 12823	4.9	6
41	Prediction of a Superhard Carbon-Rich CN Compound Comparable to Diamond. *Journal of Physical Chemistry C*, **2015**, 119, 28614-28619	3.8	23
40	Exotic stable cesium polynitrides at high pressure. *Scientific Reports*, **2015**, 5, 16902	4.9	41
39	Nitrogen Backbone Oligomers. *Scientific Reports*, **2015**, 5, 13239	4.9	27
38	Mechanisms for pressure-induced crystal-crystal transition, amorphization, and devitrification of SnI4. *Journal of Chemical Physics*, **2015**, 143, 164508	3.9	8
37	Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide. *Scientific Reports*, **2015**, 5, 8761	4.9	16
36	Prediction of novel crystal structures and superconductivity of compressed HBr. *RSC Advances*, **2015**, 5, 45812-45816	3.7	6
35	Pressure-stabilized superconductive yttrium hydrides. *Scientific Reports*, **2015**, 5, 9948	4.9	184
34	Structures of the metallic and superconducting high pressure phases of solid CS2. *Scientific Reports*, **2015**, 5, 10458	4.9	14

33	Crystalline LiN5 Predicted from First-Principles as a Possible High-Energy Material. *Journal of Physical Chemistry Letters*, **2015**, 6, 2363-6	6.4	98
32	Stable structures of He and H2O at high pressure. *Physical Review B*, **2015**, 91,	3.3	43
31	N2H: a novel polymeric hydronitrogen as a high energy density material. *Journal of Materials Chemistry A*, **2015**, 3, 4188-4194	13	42
30	Superhard BC(3) in cubic diamond structure. *Physical Review Letters*, **2015**, 114, 015502	7.4	147
29	Metallization and superconductivity of BeH2 under high pressure. *Journal of Chemical Physics*, **2014** , 140, 124707	3.9	39
28	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. *Nature Chemistry*, **2014**, 6, 644-8	17.6	314
27	Self-assembled ultrathin nanotubes on diamond (100) surface. *Nature Communications*, **2014**, 5, 3666	17.4	133
26	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. *Journal of Physical Chemistry C*, **2014**, 118, 11902-11905	3.8	7
25	The metallization and superconductivity of dense hydrogen sulfide. *Journal of Chemical Physics*, **2014**, 140, 174712	3.9	481
24	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. *Chemical Science*, **2014**, 5, 3936-3940	9.4	19
23	Structural and mechanical properties of platinum carbide. *Inorganic Chemistry*, **2014**, 53, 5797-802	5.1	16
22	Direct band gap silicon allotropes. *Journal of the American Chemical Society*, **2014**, 136, 9826-9	16.4	120
21	Superhard sp 3 carbon allotrope: Ab initio calculations. *Europhysics Letters*, **2014**, 108, 46006	1.6	4
20	Hardness of FeB4: density functional theory investigation. *Journal of Chemical Physics*, **2014**, 140, 174505	3.9	67
19	Novel high-pressure crystal structures of boron trifluoride. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 1094-1098	3.9	2
18	Orthorhombic C32: a novel superhard sp3 carbon allotrope. *Physical Chemistry Chemical Physics*, **2013**, 15, 14120-5	3.6	52
17	Proton or deuteron transfer in phase IV of solid hydrogen and deuterium. *Physical Review Letters*, **2013**, 110, 025903	7.4	57
16	Anomalous Melting Behavior of Solid Hydrogen at High Pressures. *Journal of Physical Chemistry C*, **2013**, 117, 11873-11877	3.8	10

15	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. *Physical Review B*, **2013**, 88,	3.3	52
14	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
13	Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. *Journal of Chemical Physics*, **2012**, 137, 184502	3.9	13
12	A novel low compressible and superhard carbon nitride: body-centered tetragonal CN2. *Physical Chemistry Chemical Physics*, **2012**, 14, 13081-7	3.6	91
11	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. *Journal of Physical Chemistry C*, **2012**, 116, 9221-9226	3.8	67
10	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
9	Room-temperature structures of solid hydrogen at high pressures. *Journal of Chemical Physics*, **2012**, 137, 074501	3.9	64
8	Predicting two-dimensional boron-carbon compounds by the global optimization method. *Journal of the American Chemical Society*, **2011**, 133, 16285-90	16.4	209
7	First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium. *Journal of Applied Physics*, **2011**, 109, 063514	2.5	50
6	Melting curve of lithium from quantum molecular-dynamics simulations. *Europhysics Letters*, **2011**, 95, 56004	1.6	8
5	High pressure partially ionic phase of water ice. *Nature Communications*, **2011**, 2, 563	17.4	201
4	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
3	Superhard polymorphs of diamond-like BC7. *Solid State Communications*, **2011**, 151, 716-719	1.6	34
2	Design of Superhard Ternary Compounds under High Pressure: SiC2N4 and Si2CN4. *Journal of Physical Chemistry C*, **2010**, 114, 8609-8613	3.8	17
1	Anomalous optical and electronic properties of dense sodium. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 4458-4464	2.3	