Hanyu Liu

List of Publications by Year
in descending order

191 papers	9,853 citations	38660 50 h-index	39575 94 g-index
197 all docs	197 docs citations	197 times ranked	5434 citing authors

#	Article	IF	Citations
1	Potential high- <i> T _c </i> 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.	3.3	651
2	The metallization and superconductivity of dense hydrogen sulfide. Journal of Chemical Physics, 2014, 140, 174712.	1.2	612
3	A General Route to Prepare Lowâ€Rutheniumâ€Content Bimetallic Electrocatalysts for pHâ€Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. Angewandte Chemie - International Edition, 2020, 59, 1718-1726.	7.2	452
4	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	2.9	377
5	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. Nature Chemistry, 2014, 6, 644-648.	6.6	369
6	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
7	Pressure-stabilized superconductive yttrium hydrides. Scientific Reports, 2015, 5, 9948.	1.6	257
8	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. Physical Review Letters, 2019, 123, 097001.	2.9	255
9	Predicting Two-Dimensional Boronâ€"Carbon Compounds by the Global Optimization Method. Journal of the American Chemical Society, 2011, 133, 16285-16290.	6.6	242
10	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	13.7	222
11	High pressure partially ionic phase of water ice. Nature Communications, 2011, 2, 563.	5.8	208
12	Synthesis and Stability of Lanthanum Superhydrides. Angewandte Chemie - International Edition, 2018, 57, 688-692.	7.2	202
13	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
14	Self-assembled ultrathin nanotubes on diamond (100) surface. Nature Communications, 2014, 5, 3666.	5.8	164
15	A high-entropy metal oxide as chemical anchor of polysulfide for lithium-sulfur batteries. Energy Storage Materials, 2019, 23, 678-683.	9.5	163
16	Direct Band Gap Silicon Allotropes. Journal of the American Chemical Society, 2014, 136, 9826-9829.	6.6	151
17	High-Temperature Superconducting Phase in Clathrate Calcium Hydride <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CaH</mml:mi></mml:mrow><mml:mrow><mml:mn>6</mml:mn>< up to 215ÂK at a Pressure of 172ÂGPa. Physical Review Letters, 2022, 128, 167001.	2.9	149
18	Compressed sodalite-like MgH₆ as a potential high-temperature superconductor. RSC Advances, 2015, 5, 59292-59296.	1.7	147

#	Article	IF	Citations
19	Crystalline LiN₅ Predicted from First-Principles as a Possible High-Energy Material. Journal of Physical Chemistry Letters, 2015, 6, 2363-2366.	2.1	145
20	Toward ultrafast lithium ion capacitors: A novel atomic layer deposition seeded preparation of Li4Ti5O12/graphene anode. Nano Energy, 2017, 36, 46-57.	8.2	138
21	High-Energy Density and Superhard Nitrogen-Rich B-N Compounds. Physical Review Letters, 2015, 115, 105502.	2.9	132
22	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	2.9	132
23	Route to high-energy density polymeric nitrogen t-N via Heâˆ’N compounds. Nature Communications, 2018, 9, 722.	5.8	131
24	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
25	A novel low compressible and superhard carbon nitride: Body-centered tetragonal CN2. Physical Chemistry Chemical Physics, 2012, 14, 13081.	1.3	108
26	Route to high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:ma superconductivity via <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml -intercalated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="n	1.1	98
27	Stable Calcium Nitrides at Ambient and High Pressures. Inorganic Chemistry, 2016, 55, 7550-7555.	1.9	88
28	Dynamics and superconductivity in compressed lanthanum superhydride. Physical Review B, 2018, 98, .	1.1	85
29	Hardness of FeB4: Density functional theory investigation. Journal of Chemical Physics, 2014, 140, 174505.	1.2	80
30	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
31	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. Journal of Physical Chemistry C, 2012, 116, 9221-9226.	1.5	78
32	Crystal Structure and Superconductivity of PH₃ at High Pressures. Journal of Physical Chemistry C, 2016, 120, 3458-3461.	1.5	78
33	Two-dimensional boronâ€“nitrogenâ€“carbon monolayers with tunable direct band gaps. Nanoscale, 2015, 7, 12023-12029.	2.8	74
34	A New Allotrope of Nitrogen as High-Energy Density Material. Journal of Physical Chemistry A, 2016, 120, 2920-2925.	1.1	73
35	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	1.6	71
36	Room-temperature structures of solid hydrogen at high pressures. Journal of Chemical Physics, 2012, 137, 074501.	1.2	69

#	Article	IF	Citations
37	Rare Helium-Bearing Compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>FeO</mml:mi></mml:mrow><mml:mrow><mml:mn> Stabilized at Deep-Earth Conditions. Physical Review Letters, 2018, 121, 255703.	2.9	68
38	First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium. Journal of Applied Physics, 2011, 109, .	1.1	66
39	Prediction of high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi></mml:msub></mml:ma superconductivity in ternary lanthanum borohydrides. Physical Review B, 2021, 104, .	1.1	66
40	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. Physical Review B, 2013, 88, .	1.1	63
41	Orthorhombic C32: a novel superhard sp3 carbon allotrope. Physical Chemistry Chemical Physics, 2013, 15, 14120.	1.3	62
42	Carbon-boron clathrates as a new class of sp ³ -bonded framework materials. Science Advances, 2020, 6, eaay8361.	4.7	61
43	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
44	Proton or Deuteron Transfer in Phase IV of Solid Hydrogen and Deuterium. Physical Review Letters, 2013, 110, 025903.	2.9	59
45	Exotic stable cesium polynitrides at high pressure. Scientific Reports, 2015, 5, 16902.	1.6	58
46	Stable structures of He and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>at high pressure. Physical Review B, 2015, 91, .	1.1	58
47	Divergent synthesis routes and superconductivity of ternary hydride<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgSiH</mml:mi><mml:mn>6</mml:mn></mml:msub> high pressure. Physical Review B, 2017, 96, .	1.1	57
48	Electron-phonon coupling mechanisms for hydrogen-rich metals at high pressure. Physical Review B, 2017, 96, .	1.1	56
49	Prediction of Stable Iron Nitrides at Ambient and High Pressures with Progressive Formation of New Polynitrogen Species. Chemistry of Materials, 2018, 30, 8476-8485.	3.2	56
50	BC8 Silicon (Si-III) is a Narrow-Gap Semiconductor. Physical Review Letters, 2017, 118, 146601.	2.9	53
51	Metallization and superconductivity of BeH2 under high pressure. Journal of Chemical Physics, 2014, 140, 124707.	1.2	50
52	Structure and Electronic Properties of Fe₂SH₃ Compound under High Pressure. Inorganic Chemistry, 2016, 55, 11434-11439.	1.9	50
53	N₂H: a novel polymeric hydronitrogen as a high energy density material. Journal of Materials Chemistry A, 2015, 3, 4188-4194.	5.2	49
54	Two-Dimensional C₄N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. Journal of Physical Chemistry C, 2017, 121, 2669-2674.	1.5	49

#	Article	IF	Citations
55	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. Journal of Physical Chemistry Letters, 2020, 11, 8710-8720.	2.1	45
56	Janus CoN/Co cocatalyst in porous N-doped carbon: toward enhanced catalytic activity for hydrogen evolution. Catalysis Science and Technology, 2018, 8, 3695-3703.	2.1	42
57	A General Route to Prepare Lowâ€Rutheniumâ€Content Bimetallic Electrocatalysts for pHâ€Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. Angewandte Chemie, 2020, 132, 1735-1743.	1.6	40
58	Chemically Tuning Stability and Superconductivity of Pâ€"H Compounds. Journal of Physical Chemistry Letters, 2020, 11, 935-939.	2.1	40
59	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	1.2	40
60	Melting and High <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>P</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>T</mml:mi></mml:mrow></mml:math> Transitions of Hydrogen up to 300ÂGPa. Physical Review Letters, 2017, 119, 075302.	2.9	39
61	Synthesis of Xenon and Iron-Nickel Intermetallic Compounds at Earthâ€™s Core Thermodynamic Conditions. Physical Review Letters, 2018, 120, 096001.	2.9	39
62	Superhard polymorphs of diamond-like. Solid State Communications, 2011, 151, 716-719.	0.9	38
63	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. Journal of Physical Chemistry C, 2018, 122, 19370-19378.	1.5	38
64	Superconductivity in dense carbon-based materials. Physical Review B, 2016, 93, .	1.1	37
65	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. Matter and Radiation at Extremes, 2020, 5, .	1.5	37
66	Single-bonded allotrope of nitrogen predicted at high pressure. Physical Review B, 2017, 96, .	1.1	36
67	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. Chemistry of Materials, 2020, 32, 459-467.	3.2	35
68	Pressure-Induced Structures and Properties in Indium Hydrides. Inorganic Chemistry, 2015, 54, 9924-9928.	1.9	34
69	Unraveling Stable Vanadium Tetraboride and Triboride by First-Principles Computations. Journal of Physical Chemistry C, 2015, 119, 21649-21657.	1.5	33
70	First-principles study of crystal structures and superconductivity of ternary <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YSH</mml:mi><mml:mn>6</mml:mn></mml:msub></mm and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaSH</mml:mi><mml:mn>6</mml:mn></mml:msub></m at high pressures. Physical Review B, 2019, 100, .	1.1	33
71	Prediction of Above-Room-Temperature Superconductivity in Lanthanide/Actinide Extreme Superhydrides. Journal of the American Chemical Society, 2022, 144, 13394-13400.	6.6	33
72	Nb-H system at high pressures and temperatures. Physical Review B, 2017, 95, .	1.1	32

#	Article	IF	Citations
73	Nitrogen Backbone Oligomers. Scientific Reports, 2015, 5, 13239.	1.6	28
74	Crystal structures and dynamical properties of dense CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11110-11115.	3.3	28
75	Bi and Sn Co-doping Enhanced Thermoelectric Properties of Cu₃SbS₄ Materials with Excellent Thermal Stability. ACS Applied Materials & Interfaces, 2020, 12, 8271-8279.	4.0	28
76	Prediction of a Superhard Carbon-Rich Câ€“N Compound Comparable to Diamond. Journal of Physical Chemistry C, 2015, 119, 28614-28619.	1.5	26
77	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. Scientific Reports, 2015, 5, 11381.	1.6	26
78	Dense Hydrocarbon Structures at Megabar Pressures. Journal of Physical Chemistry Letters, 2016, 7, 4218-4222.	2.1	26
79	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.		26
80	Synthesis of Bulk BC8 Silicon Allotrope by Direct Transformation and Reduced-Pressure Chemical Pathways. Inorganic Chemistry, 2016, 55, 8943-8950.	1.9	25
81	Predicting the structure and stability of titanium oxide electrides. Npj Computational Materials, 2018, 4, .	3.5	25
82	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
83	Crystal Structures and Properties of Iron Hydrides at High Pressure. Journal of Physical Chemistry C, 2018, 122, 24262-24269.	1.5	24
84	Semiconducting cubic titanium nitride in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Th</mml:mi><mml:mn>3</mml:mn></mml: mathvariant="normal">P</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>structure. Physical Review Materials, 2018, 2, .	0.9	24
85	A new high-pressure polymeric nitrogen phase in potassium azide. RSC Advances, 2015, 5, 11825-11830.	1.7	23
86	Stability of H3O 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
87	Synthesis and Stability of Lanthanum Superhydrides. Angewandte Chemie, 2018, 130, 696-700.	1.6	22
88	Pressure stabilization of long-missing bare C6 hexagonal rings in binary sesquicarbides. Chemical Science, 2014, 5, 3936-3940.	3.7	21
89	Design of Superhard Ternary Compounds under High Pressure: SiC₂N₄and Si₂CN₄. Journal of Physical Chemistry C, 2010, 114, 8609-8613.	1.5	20
90	Synthesis and stability of tantalum hydride at high pressures. Physical Review B, 2019, 99, .	1.1	20

#	Article	IF	Citations
91	Structure and superconductivity in compressed Li-Si-H compounds: Density functional theory calculations. Physical Review B, 2020, 102, .	1.1	20
92	Structural and Mechanical Properties of Platinum Carbide. Inorganic Chemistry, 2014, 53, 5797-5802.	1.9	19
93	Structures of the metallic and superconducting high pressure phases of solid CS2. Scientific Reports, 2015, 5, 10458.	1.6	18
94	Crystal Structures and Chemical Bonding of Magnesium Carbide at High Pressure. Journal of Physical Chemistry C, 2015, 119, 23168-23174.	1.5	18
95	Direct H-He chemical association in superionic FeO2H2He at Deep-Earth conditions. National Science Review, 0, , .	4.6	18
96	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. Scientific Reports, 2015, 5, 13039.	1.6	17
97	Polymerization of Nitrogen in Ammonium Azide at High Pressures. Journal of Physical Chemistry C, 2015, 119, 25268-25272.	1.5	17
98	Quantum and Classical Proton Diffusion in Superconducting Clathrate Hydrides. Physical Review Letters, 2021, 126, 117002.	2.9	17
99	Path to high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi mathvariant="normal">c</mml:mi></mml:msub></mml:math> superconductivity via Rb substitution of guest metal atoms in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Sr</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant	1.1	17
100	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.	2.8	16
101	Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide. Scientific Reports, 2015, 5, 8761.	1.6	16
102	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. Journal of Physical Chemistry Letters, 2016, 7, 4898-4904.	2.1	16
103	Superconductive Sodium Carbides with Pentagon Carbon at High Pressures. Journal of Physical Chemistry Letters, 2021, 12, 5850-5856.	2.1	16
104	Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. Journal of Chemical Physics, 2012, 137, 184502.	1.2	15
105	High pressure polyhydrides of molybdenum: A first-principles study. Solid State Communications, 2016, 239, 14-19.	0.9	15
106	Crystal structures and superconductivity of technetium hydrides under pressure. Physical Chemistry Chemical Physics, 2016, 18, 28791-28796.	1.3	15
107	Different evolutionary pathways from B4 to B1 phase in AlN and InN: metadynamics investigations. Journal of Physics Condensed Matter, 2016, 28, 205403.	0.7	15
108	Phase transition and superconductivity in ReS2, ReSe2 and ReTe2. Physical Chemistry Chemical Physics, 2018, 20, 29472-29479.	1.3	15

#	Article	IF	Citations
109	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	1.1	15
110	Pressure-induced polyamorphism in a main-group metallic glass. Physical Review B, 2016, 94, .	1.1	14
111	Hard BN Clathrate Superconductors. Journal of Physical Chemistry Letters, 2019, 10, 2554-2560.	2.1	14
112	Anomalous Melting Behavior of Solid Hydrogen at High Pressures. Journal of Physical Chemistry C, 2013, 117, 11873-11877.	1.5	13
113	Mechanisms for pressure-induced crystal-crystal transition, amorphization, and devitrification of SnI4. Journal of Chemical Physics, 2015, 143, 164508.	1.2	13
114	Experimental clathrate superhydrides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>EuH</mml:mi><mml:mn>6</mml:mn></mml:msub></mm and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>EuH</mml:mi><mml:mn>9</mml:mn></mml:msub></mm at extreme pressure conditions. Physical Review Research, 2021, 3, .	1.3	13
115	Unexpected Semimetallic BiS₂ at High Pressure and High Temperature. Journal of Physical Chemistry Letters, 2018, 9, 5785-5791.	2.1	12
116	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	3.5	12
117	Synthesis of new nickel hydrides at high pressure. Physical Review Materials, 2018, 2, .	0.9	12
118	Superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">H</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:math> doped with light elements. Physical Review Research, 2021, 3, .	1.3	12
119	Design and synthesis of clathrate <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaB</mml:mi><mml:mn>8</mml:mn></mml:msub></mm with superconductivity. Physical Review B, 2021, 104, .	1.1	12
120	Prediction of the Xeâ€"He binary phase diagram at high pressures. Chemical Physics Letters, 2015, 640, 115-118.	1.2	11
121	Predicted two-dimensional electrides: Lithiumâ€"carbon monolayer sheet. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 2511-2514.	0.9	11
122	Theoretical investigation of the valence states in Au <i>via</i> the Auâ€"F compounds under high pressure. Physical Chemistry Chemical Physics, 2019, 21, 17621-17627.	1.3	11
123	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	2.4	11
124	Theoretical design of two-dimensional carbon nitrides. Nanotechnology, 2020, 31, 495707.	1.3	11
125	Competition among Refined Hollow Structures in Schiff Base Polymer Derived Carbon Microspheres. Nano Letters, 2022, 22, 3691-3698.	4.5	11
126	Decomposition and Recombination of Binary Interalkali Na₂K at High Pressures. Journal of Physical Chemistry Letters, 2019, 10, 3006-3012.	2.1	10

#	Article	IF	Citations
127	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. Physical Review B, 2019, 99, .	1.1	10
128	Pressure-Tuned Core/Shell Configuration Transition of Shell Thickness-Dependent CdSe/CdS Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 920-926.	2.1	10
129	Stable Structures and Superconductivity in a Yâ€“Si System under High Pressure. Journal of Physical Chemistry Letters, 2021, 12, 10388-10393.	2.1	10
130	Orthorhombic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScB</mml:mi><mml:mn>3</mml:mn></mml:msub></mm and hexagonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScB</mml:mi><mml:mn>6</mml:mn></mml:msub></mm with high hardness. Physical Review B, 2022, 105, .	1.1	10
131	Pressure-induced superconductivity and structure phase transition in Pt2HgSe3. Npj Quantum Materials, 2021, 6, .	1.8	10
132	Melting curve of lithium from quantum molecular-dynamics simulations. Europhysics Letters, 2011, 95, 56004.	0.7	9
133	Shock compression behavior of a mixture of cubic and hexagonal boron nitride. Journal of Applied Physics, 2018, 123, .	1.1	9
134	Pressure-induced decomposition of binary lanthanum intermetallic compounds. Physical Review B, 2020, 101, .	1.1	9
135	The electrical conductivity of Al2O3 under shock-compression. Scientific Reports, 2015, 5, 12823.	1.6	8
136	Prediction of Hostâ€“Guest Naâ€“Fe Intermetallics at High Pressures. Inorganic Chemistry, 2016, 55, 7026-7032.	1.9	8
137	High-pressure crystal structures of TaAs from first-principles calculations. Solid State Communications, 2016, 240, 37-40.	0.9	8
138	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiBC₁₁ and Li₂B₂C₁₀. RSC Advances, 2016, 6, 52695-52699.	1.7	8
139	Carbon network evolution from dimers to sheets in superconducting ytrrium dicarbide under pressure. Communications Chemistry, 2018, 1, .	2.0	8
140	Predicted Stable Structures of the Liâ€“Ag System at High Pressures. Journal of Physical Chemistry Letters, 2021, 12, 1671-1675.	2.1	8
141	Exploring the structures and properties of nickel silicides at the pressures of the Earthâ€™s core. Physical Chemistry Chemical Physics, 2021, 23, 14671-14677.	1.3	8
142	Superhard sp 3 carbon allotrope: Ab initio calculations. Europhysics Letters, 2014, 108, 46006.	0.7	7
143	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. Journal of Physical Chemistry C, 2014, 118, 11902-11905.	1.5	7
144	Structures and stability of novel transition-metal<mml:math		

#	Article	IF	Citations
145	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.	4.2	7
146	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of Na4Ge13. Inorganic Chemistry, 2018, 57, 2002-2012.	1.9	7
147	Crystal Structures and Electronic Properties of Xeâ€"Cl Compounds at High Pressure. Journal of Physical Chemistry C, 2018, 122, 2941-2950.	1.5	7
148	Predicted CsSi compound: a promising material for photovoltaic applications. Physical Chemistry Chemical Physics, 2020, 22, 11578-11582.	1.3	7
149	<i>Ab initio</i> high-throughput screening of transition metal double chalcogenide monolayers as highly efficient bifunctional catalysts for photochemical and photoelectrochemical water splitting. Journal of Materials Chemistry A, 2022, 10, 14060-14069.	5.2	7
150	Prediction of novel crystal structures and superconductivity of compressed HBr. RSC Advances, 2015, 5, 45812-45816.	1.7	6
151	High-pressure phase transitions of nitinol NiTi to a semiconductor with an unusual topological structure. Physical Review B, 2018, 97, .	1.1	6
152	Superconducting TaH5 at high pressure. New Journal of Physics, 2019, 21, 123009.	1.2	6
153	Novel high-pressure structure and superconductivity of titanium trisulfide. Computational Materials Science, 2019, 158, 192-196.	1.4	6
154	Open questions on the high-pressure chemistry of the noble gases. Communications Chemistry, 2022, 5, .	2.0	6
155	Low-Pressure Electrochemical Synthesis of Complex High-Pressure Superconducting Superhydrides. Physical Review Letters, 2022, 128, 186001.	2.9	6
156	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. Scientific Reports, 2016, 6, 18918.	1.6	5
157	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.	5.0	5
158	Effect of the Inherent Structure of Rh Nanocrystals on the Hydriding Behavior under Pressure. Journal of Physical Chemistry Letters, 2019, 10, 774-779.	2.1	5
159	Superconducting thorium hydrides under high pressure. Solid State Communications, 2020, 309, 113820.	0.9	5
160	Potassium-activated anionic copper and covalent Cuâ€"Cu bonding in compressed Kâ€"Cu compounds. Journal of Chemical Physics, 2021, 154, 134708.	1.2	5
161	Retainable Superconductivity and Structural Transition in 1T-TaSe2 Under High Pressure. Inorganic Chemistry, 2021, 60, 11385-11393.	1.9	5
162	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. Chemistry - A European Journal, 2021, 27, 17420-17427.	1.7	5

#	Article	IF	Citations
163	Novel Valence Transition in Elemental Metal Europium around 80ÂGPa. Physical Review Letters, 2022, 129, .	2.9	5
164	Ambient-Pressure Polymerization of Carbon Anions in the High-Pressure Phase Mg₂C. Inorganic Chemistry, 2015, 54, 10761-10765.	1.9	4
165	Predicted lithiumâ€"iron compounds under high pressure. RSC Advances, 2016, 6, 66721-66728.	1.7	4
166	First principles study of LiAlO₂: new dense monoclinic phase under high pressure. Journal of Physics Condensed Matter, 2018, 30, 115401.	0.7	4
167	Theoretical research on novel orthorhombic tungsten dinitride from first principles calculations. RSC Advances, 2018, 8, 9272-9276.	1.7	4
168	Pressure-induced structural modulations in coesite. Physical Review B, 2018, 98, .	1.1	4
169	Prediction of a stable helium-hydrogen compound: First-principles simulations. Physical Review B, 2021, 104, .	1.1	4
170	Phase transition and electronic properties of barium fluoride at high pressure. Solid State Communications, 2022, 342, 114597.	0.9	4
171	Theory-directed discovery of high-temperature superconductivity in clathrate hydrides at high pressure. Innovation(China), 2022, 3, 100226.	5.2	4
172	High-pressure modulated structures in beryllium chalcogenides. Physical Review B, 2019, 100, .	1.1	3
173	Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. Physical Chemistry Chemical Physics, 2021, 23, 21544-21553.	1.3	3
174	Crystal structures and superconductivity of carbonaceous sulfur hydrides at pressures up to 300 GPa. Physical Review B, 2022, 105, .	1.1	3
175	Novel high-pressure crystal structures of boron trifluoride. Journal of Physics and Chemistry of Solids, 2014, 75, 1094-1098.	1.9	2
176	Crystal Structures of CaB₃N₃ at High Pressures. Inorganic Chemistry, 2017, 56, 7449-7453.	1.9	2
177	Computational prediction of aâ€‰â€‰+4 oxidation state in Au via compressed AuO2 compound. Journal of Physics Condensed Matter, 2020, 32, 015402.	0.7	2
178	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	1.1	2
179	Superconductive hydrogen-rich compounds under high pressure. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	2
180	Metadynamics investigations of the AlN/GaN superlattice. Europhysics Letters, 2016, 114, 46002.	0.7	1

#	Article	IF	Citations
181	Reply to Datchi et al.: Recovered phase CO2-V at low temperature and a newly predicted 3D-extended CO2phase. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E658-E659.	3.3	1
182	Novel boron channel-based structure of boron carbide at high pressures. Journal of Physics Condensed Matter, 2017, 29, 455401.	0.7	1
183	First-principles molecular dynamics simulations of single nitrogen bond structures in a N2H2 system under pressure. Solid State Communications, 2019, 290, 27-30.	0.9	1
184	Oxysulfide Li2BeSO: A potential new material for solid electrolyte predicted from first principles. Journal of Alloys and Compounds, 2020, 818, 152844.	2.8	1
185	A new intermediate phase in compressed nitinol. Journal of Alloys and Compounds, 2020, 817, 153234.	2.8	1
186	Superconductivity in metal intercalated graphite-like boron-carbon-nitrogen. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 402, 127348.	0.9	1
187	Prediction of stable Cu structure and phase transition mechanism at ultra-high pressure: A comprehensive properties characterization by DFT calculation. Physica B: Condensed Matter, 2022, 625, 413538.	1.3	1
188	Structural characteristics and elasticities of coesite and coesite-II at high pressure. New Journal of Physics, 2020, 22, 093044.	1.2	1
189	High-Pressure Structures and Superconductivity of Barium Iodide. Materials, 2022, 15, 522.	1.3	1
190	High pressure nanoarchitectonics and metallization of barium chloride and barium bromide. Journal of Physics Condensed Matter, 2022, 34, 294002.	0.7	1
191	Anomalous optical and electronic properties of dense sodium. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 4458-4464.	0.9	0