

Hanyu Liu

List of Publications by Citations

Source: <https://exaly.com/author-pdf/8327380/hanyu-liu-publications-by-citations.pdf>

Version: 2024-04-23

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	The metallization and superconductivity of dense hydrogen sulfide. <i>Journal of Chemical Physics</i> , 2014 , 140, 174712	3.9	481
175	Potential high- superconducting lanthanum and yttrium hydrides at high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 6990-6995	11.5	387
174	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. <i>Nature Chemistry</i> , 2014 , 6, 644-8	17.6	314
173	High-pressure hydrogen sulfide from first principles: a strongly anharmonic phonon-mediated superconductor. <i>Physical Review Letters</i> , 2015 , 114, 157004	7.4	299
172	A General Route to Prepare Low-Ruthenium-Content Bimetallic Electrocatalysts for pH-Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 1718-1726	16.4	250
171	An effective structure prediction method for layered materials based on 2D particle swarm optimization algorithm. <i>Journal of Chemical Physics</i> , 2012 , 137, 224108	3.9	223
170	Predicting two-dimensional boron-carbon compounds by the global optimization method. <i>Journal of the American Chemical Society</i> , 2011 , 133, 16285-90	16.4	209
169	High pressure partially ionic phase of water ice. <i>Nature Communications</i> , 2011 , 2, 563	17.4	201
168	Pressure-stabilized superconductive yttrium hydrides. <i>Scientific Reports</i> , 2015 , 5, 9948	4.9	184
167	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. <i>Nature</i> , 2016 , 532, 81-4	50.4	165
166	Superhard BC(3) in cubic diamond structure. <i>Physical Review Letters</i> , 2015 , 114, 015502	7.4	147
165	Synthesis and Stability of Lanthanum Superhydrides. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 688-692	16.4	134
164	Self-assembled ultrathin nanotubes on diamond (100) surface. <i>Nature Communications</i> , 2014 , 5, 3666	17.4	133
163	Route to a Superconducting Phase above Room Temperature in Electron-Doped Hydride Compounds under High Pressure. <i>Physical Review Letters</i> , 2019 , 123, 097001	7.4	125
162	Direct band gap silicon allotropes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 9826-9	16.4	120
161	Toward ultrafast lithium ion capacitors: A novel atomic layer deposition seeded preparation of Li4Ti5O12/graphene anode. <i>Nano Energy</i> , 2017 , 36, 46-57	17.1	115
160	High-Energy Density and Superhard Nitrogen-Rich B-N Compounds. <i>Physical Review Letters</i> , 2015 , 115, 105502	7.4	106

159	Compressed sodalite-like MgH ₆ as a potential high-temperature superconductor. <i>RSC Advances</i> , 2015 , 5, 59292-59296	3.7	104
158	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. <i>Physical Review Letters</i> , 2016 , 116, 057002	7.4	104
157	Crystalline LiN ₅ Predicted from First-Principles as a Possible High-Energy Material. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 2363-6	6.4	98
156	Dissociation products and structures of solid H ₂ S at strong compression. <i>Physical Review B</i> , 2016 , 93,	3.3	96
155	Route to high-energy density polymeric nitrogen t-N via He-N compounds. <i>Nature Communications</i> , 2018 , 9, 722	17.4	95
154	A novel low compressible and superhard carbon nitride: body-centered tetragonal CN ₂ . <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 13081-7	3.6	91
153	A high-entropy metal oxide as chemical anchor of polysulfide for lithium-sulfur batteries. <i>Energy Storage Materials</i> , 2019 , 23, 678-683	19.4	81
152	Hardness of FeB ₄ : density functional theory investigation. <i>Journal of Chemical Physics</i> , 2014 , 140, 174505.9	5.9	67
151	Quasi-Molecular and Atomic Phases of Dense Solid Hydrogen. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 9221-9226	3.8	67
150	Room-temperature structures of solid hydrogen at high pressures. <i>Journal of Chemical Physics</i> , 2012 , 137, 074501	3.9	64
149	Two-dimensional boron-nitrogen-carbon monolayers with tunable direct band gaps. <i>Nanoscale</i> , 2015 , 7, 12023-9	7.7	63
148	Crystal Structure and Superconductivity of PH ₃ at High Pressures. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 3458-3461	3.8	59
147	Proton or deuteron transfer in phase IV of solid hydrogen and deuterium. <i>Physical Review Letters</i> , 2013 , 110, 025903	7.4	57
146	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. <i>Scientific Reports</i> , 2015 , 5, 15433	4.9	56
145	Superhard and superconductive polymorphs of diamond-like BC ₃ . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011 , 375, 771-774	2.3	53
144	Dynamics and superconductivity in compressed lanthanum superhydride. <i>Physical Review B</i> , 2018 , 98,	3.3	53
143	Orthorhombic C ₃₂ : a novel superhard sp ³ carbon allotrope. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 14120-5	3.6	52
142	Theoretical study of the ground-state structures and properties of niobium hydrides under pressure. <i>Physical Review B</i> , 2013 , 88,	3.3	52

141	Stable Calcium Nitrides at Ambient and High Pressures. <i>Inorganic Chemistry</i> , 2016 , 55, 7550-5	5.1	51
140	First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium. <i>Journal of Applied Physics</i> , 2011 , 109, 063514	2.5	50
139	A New Allotrope of Nitrogen as High-Energy Density Material. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 2920-5	2.8	49
138	Route to high-T _c superconductivity via CH ₄ -intercalated H ₃ S hydride perovskites. <i>Physical Review B</i> , 2020 , 101,	3.3	45
137	Stable structures of He and H ₂ O at high pressure. <i>Physical Review B</i> , 2015 , 91,	3.3	43
136	N ₂ H: a novel polymeric hydronitrogen as a high energy density material. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 4188-4194	1.3	42
135	Exotic stable cesium polynitrides at high pressure. <i>Scientific Reports</i> , 2015 , 5, 16902	4.9	41
134	Metallization and superconductivity of BeH ₂ under high pressure. <i>Journal of Chemical Physics</i> , 2014 , 140, 124707	3.9	39
133	Rare Helium-Bearing Compound FeO ₂ He Stabilized at Deep-Earth Conditions. <i>Physical Review Letters</i> , 2018 , 121, 255703	7.4	38
132	Two-Dimensional C ₄ N Global Minima: Unique Structural Topologies and Nanoelectronic Properties. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 2669-2674	3.8	37
131	Electron-phonon coupling mechanisms for hydrogen-rich metals at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	35
130	Structure and Electronic Properties of FeSH Compound under High Pressure. <i>Inorganic Chemistry</i> , 2016 , 55, 11434-11439	5.1	35
129	BC ₈ Silicon (Si-III) is a Narrow-Gap Semiconductor. <i>Physical Review Letters</i> , 2017 , 118, 146601	7.4	35
128	Superhard polymorphs of diamond-like BC ₇ . <i>Solid State Communications</i> , 2011 , 151, 716-719	1.6	34
127	Melting and High P-T Transitions of Hydrogen up to 300 GPa. <i>Physical Review Letters</i> , 2017 , 119, 075302	7.4	33
126	Prediction of Stable Iron Nitrides at Ambient and High Pressures with Progressive Formation of New Polynitrogen Species. <i>Chemistry of Materials</i> , 2018 , 30, 8476-8485	9.6	33
125	Divergent synthesis routes and superconductivity of ternary hydride MgSiH ₆ at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	32
124	Janus CoN/Co cocatalyst in porous N-doped carbon: toward enhanced catalytic activity for hydrogen evolution. <i>Catalysis Science and Technology</i> , 2018 , 8, 3695-3703	5.5	31

123	Synthesis of Xenon and Iron-Nickel Intermetallic Compounds at Earth's Core Thermodynamic Conditions. <i>Physical Review Letters</i> , 2018 , 120, 096001	7.4	28
122	Nb-H system at high pressures and temperatures. <i>Physical Review B</i> , 2017 , 95,	3.3	27
121	New Calcium Hydrides with Mixed Atomic and Molecular Hydrogen. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 19370-19378	3.8	27
120	Single-bonded allotrope of nitrogen predicted at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	27
119	Nitrogen Backbone Oligomers. <i>Scientific Reports</i> , 2015 , 5, 13239	4.9	27
118	A General Route to Prepare Low-Ruthenium-Content Bimetallic Electrocatalysts for pH-Universal Hydrogen Evolution Reaction by Using Carbon Quantum Dots. <i>Angewandte Chemie</i> , 2020 , 132, 1735-1743	3.6	26
117	Unraveling Stable Vanadium Tetraboride and Triboride by First-Principles Computations. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 21649-21657	3.8	25
116	Pressure-Induced Structures and Properties in Indium Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 9924-8	5.1	23
115	Crystal structures and dynamical properties of dense CO ₂ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 11110-11115	11.5	23
114	Prediction of a Superhard Carbon-Rich C _N Compound Comparable to Diamond. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 28614-28619	3.8	23
113	Dense Hydrocarbon Structures at Megabar Pressures. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4218-4222	6.4	22
112	Chemically Tuning Stability and Superconductivity of P-H Compounds. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 935-939	6.4	21
111	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
110	Carbon-boron clathrates as a new class of sp-bonded framework materials. <i>Science Advances</i> , 2020 , 6, eaay8361	14.3	20
109	Pressure stabilization of long-missing bare C ₆ hexagonal rings in binary sesquicarbides. <i>Chemical Science</i> , 2014 , 5, 3936-3940	9.4	19
108	First-principles study on the structural and electronic properties of metallic HfH ₂ under pressure. <i>Scientific Reports</i> , 2015 , 5, 11381	4.9	18
107	Superconductivity in dense carbon-based materials. <i>Physical Review B</i> , 2016 , 93,	3.3	18
106	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. <i>Chemistry of Materials</i> , 2020 , 32, 459-467	9.6	18

105	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 8710-8720	6.4	18
104	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2761-2766	6.4	17
103	Synthesis of Bulk BC8 Silicon Allotrope by Direct Transformation and Reduced-Pressure Chemical Pathways. <i>Inorganic Chemistry</i> , 2016 , 55, 8943-50	5.1	17
102	Design of Superhard Ternary Compounds under High Pressure: SiC ₂ N ₄ and Si ₂ CN ₄ . <i>Journal of Physical Chemistry C</i> , 2010 , 114, 8609-8613	3.8	17
101	Semiconducting cubic titanium nitride in the Th ₃ P ₄ structure. <i>Physical Review Materials</i> , 2018 , 2,	3.2	17
100	Theory-orientated discovery of high-temperature superconductors in superhydrides stabilized under high pressure. <i>Matter and Radiation at Extremes</i> , 2020 , 5, 068101	4.7	17
99	A new high-pressure polymeric nitrogen phase in potassium azide. <i>RSC Advances</i> , 2015 , 5, 11825-11830	3.7	16
98	Crystal Structures and Chemical Bonding of Magnesium Carbide at High Pressure. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 23168-23174	3.8	16
97	First-principles study of crystal structures and superconductivity of ternary YSH ₆ and LaSH ₆ at high pressures. <i>Physical Review B</i> , 2019 , 100,	3.3	16
96	Structural and mechanical properties of platinum carbide. <i>Inorganic Chemistry</i> , 2014 , 53, 5797-802	5.1	16
95	Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide. <i>Scientific Reports</i> , 2015 , 5, 8761	4.9	16
94	Predicting the structure and stability of titanium oxide electrides. <i>Npj Computational Materials</i> , 2018 , 4,	10.9	16
93	Crystal structures, stability, electronic and elastic properties of 4d and 5d transition metal monoborides: First-principles calculations. <i>Journal of Alloys and Compounds</i> , 2012 , 538, 115-124	5.7	15
92	Crystal Structures and Properties of Iron Hydrides at High Pressure. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 24262-24269	3.8	15
91	Polymerization of Nitrogen in Ammonium Azide at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 25268-25272	3.8	14
90	Bi and Sn Co-doping Enhanced Thermoelectric Properties of CuSbS Materials with Excellent Thermal Stability. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 8271-8279	9.5	14
89	Hydrogen segregation and its roles in structural stability and metallization: silane under pressure. <i>Scientific Reports</i> , 2015 , 5, 13039	4.9	14
88	Structures of the metallic and superconducting high pressure phases of solid CS ₂ . <i>Scientific Reports</i> , 2015 , 5, 10458	4.9	14

87	Synthesis and stability of tantalum hydride at high pressures. <i>Physical Review B</i> , 2019 , 99,	3.3	13
86	Different evolutionary pathways from B4 to B1 phase in AlN and InN: metadynamics investigations. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 205403	1.8	13
85	Hybrid functional study rationalizes the simple cubic phase of calcium at high pressures. <i>Journal of Chemical Physics</i> , 2012 , 137, 184502	3.9	13
84	Prediction of high-Tc superconductivity in ternary lanthanum borohydrides. <i>Physical Review B</i> , 2021 , 104,	3.3	13
83	High pressure polyhydrides of molybdenum: A first-principles study. <i>Solid State Communications</i> , 2016 , 239, 14-19	1.6	13
82	Pressure-induced polyamorphism in a main-group metallic glass. <i>Physical Review B</i> , 2016 , 94,	3.3	11
81	Phase transition and superconductivity in ReS, ReSe and ReTe. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 29472-29479	3.6	11
80	Predicted two-dimensional electrides: Lithium-carbon monolayer sheet. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2015 , 379, 2511-2514	2.3	10
79	Unexpected Semimetallic BiS at High Pressure and High Temperature. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5785-5791	6.4	10
78	Anomalous Melting Behavior of Solid Hydrogen at High Pressures. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 11873-11877	3.8	10
77	Synthesis of new nickel hydrides at high pressure. <i>Physical Review Materials</i> , 2018 , 2,	3.2	10
76	Crystal structures and superconductivity of technetium hydrides under pressure. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 28791-28796	3.6	10
75	Synthesis and Stability of Lanthanum Superhydrides. <i>Angewandte Chemie</i> , 2018 , 130, 696-700	3.6	10
74	Hard BN Clathrate Superconductors. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 2554-2560	6.4	9
73	The 2021 Room-Temperature Superconductivity Roadmap. <i>Journal of Physics Condensed Matter</i> , 2021 ,	1.8	9
72	High-Temperature Superconducting Phase in Clathrate Calcium Hydride CaH ₆ up to 215K at a Pressure of 172GPa.. <i>Physical Review Letters</i> , 2022 , 128, 167001	7.4	9
71	Stability of HO at extreme conditions and implications for the magnetic fields of Uranus and Neptune. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 5638-5643	11.5	8
70	Coexistence of Superconductivity and Superhardness in Beryllium Hexaboride Driven by Inherent Multicenter Bonding. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 4898-4904	6.4	8

69	Mechanisms for pressure-induced crystal-crystal transition, amorphization, and devitrification of SnI ₄ . <i>Journal of Chemical Physics</i> , 2015 , 143, 164508	3.9	8
68	Melting curve of lithium from quantum molecular-dynamics simulations. <i>Europhysics Letters</i> , 2011 , 95, 56004	1.6	8
67	A symmetry-orientated divide-and-conquer method for crystal structure prediction.. <i>Journal of Chemical Physics</i> , 2022 , 156, 014105	3.9	8
66	Prediction of Host-Guest Na-Fe Intermetallics at High Pressures. <i>Inorganic Chemistry</i> , 2016 , 55, 7026-32	5.1	8
65	Carbon network evolution from dimers to sheets in superconducting yttrium dicarbide under pressure. <i>Communications Chemistry</i> , 2018 , 1,	6.3	8
64	Decomposition and Recombination of Binary Interalkali NaK at High Pressures. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 3006-3012	6.4	7
63	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. <i>Physical Review B</i> , 2019 , 99,	3.3	7
62	Structures and stability of novel transition-metal (M=Co,Rh,CoandIr) borides. <i>Physical Review B</i> , 2015 , 92,	3.3	7
61	Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of NaGe. <i>Inorganic Chemistry</i> , 2018 , 57, 2002-2012	5.1	7
60	Robust Diffusive Proton Motions in Phase IV of Solid Hydrogen. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 11902-11905	3.8	7
59	Prediction of the Xe ₂ He binary phase diagram at high pressures. <i>Chemical Physics Letters</i> , 2015 , 640, 115-118	2.5	7
58	Structure and superconductivity in compressed Li-Si-H compounds: Density functional theory calculations. <i>Physical Review B</i> , 2020 , 102,	3.3	6
57	Pressure-Tuned Core/Shell Configuration Transition of Shell Thickness-Dependent CdSe/CdS Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 920-926	6.4	6
56	A combined experimental and theoretical investigation of donor and acceptor interface in efficient aqueous-processed polymer/nanocrystal hybrid solar cells. <i>Science China Chemistry</i> , 2018 , 61, 437-443	7.9	6
55	The electrical conductivity of Al ₂ O ₃ under shock-compression. <i>Scientific Reports</i> , 2015 , 5, 12823	4.9	6
54	Prediction of novel crystal structures and superconductivity of compressed HBr. <i>RSC Advances</i> , 2015 , 5, 45812-45816	3.7	6
53	Quantum and Classical Proton Diffusion in Superconducting Clathrate Hydrides. <i>Physical Review Letters</i> , 2021 , 126, 117002	7.4	6
52	High-pressure crystal structures of TaAs from first-principles calculations. <i>Solid State Communications</i> , 2016 , 240, 37-40	1.6	6

51	Machine learning metadynamics simulation of reconstructive phase transition. <i>Physical Review B</i> , 2021 , 103,	3.3	6
50	An automated predictor for identifying transition states in solids. <i>Npj Computational Materials</i> , 2020 , 6,	10.9	5
49	Shock compression behavior of a mixture of cubic and hexagonal boron nitride. <i>Journal of Applied Physics</i> , 2018 , 123, 175903	2.5	5
48	High-pressure phase transitions of nitinol NiTi to a semiconductor with an unusual topological structure. <i>Physical Review B</i> , 2018 , 97,	3.3	5
47	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. <i>Scientific Reports</i> , 2016 , 6, 18918	4.9	5
46	Theoretical investigation of the valence states in Au via the Au-F compounds under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 17621-17627	3.6	5
45	Ambient-Pressure Polymerization of Carbon Anions in the High-Pressure Phase Mg ₂ C. <i>Inorganic Chemistry</i> , 2015 , 54, 10761-5	5.1	4
44	Crystal Structures and Electronic Properties of Xe ^{II} Compounds at High Pressure. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 2941-2950	3.8	4
43	Synergistic effects of reduced graphene oxide with freeze drying tuned interfacial structure on performance of transparent and flexible supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2019 , 554, 650-657	9.3	4
42	Superhard sp ³ carbon allotrope: Ab initio calculations. <i>Europhysics Letters</i> , 2014 , 108, 46006	1.6	4
41	Pressure-induced decomposition of binary lanthanum intermetallic compounds. <i>Physical Review B</i> , 2020 , 101,	3.3	4
40	Superconductivity of H ₃ S doped with light elements. <i>Physical Review Research</i> , 2021 , 3,	3.9	4
39	Theoretical design of two-dimensional carbon nitrides. <i>Nanotechnology</i> , 2020 , 31, 495707	3.4	4
38	Predicted lithium-iron compounds under high pressure. <i>RSC Advances</i> , 2016 , 6, 66721-66728	3.7	4
37	Superconducting TaH ₅ at high pressure. <i>New Journal of Physics</i> , 2019 , 21, 123009	2.9	4
36	Predicted Stable Structures of the Li-Ag System at High Pressures. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1671-1675	6.4	4
35	Exploring the structures and properties of nickel silicides at the pressures of the Earth's core. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14671-14677	3.6	4
34	Effect of the Inherent Structure of Rh Nanocrystals on the Hydriding Behavior under Pressure. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 774-779	6.4	3

33	Predicted CsSi compound: a promising material for photovoltaic applications. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 11578-11582	3.6	3
32	Superconducting thorium hydrides under high pressure. <i>Solid State Communications</i> , 2020 , 309, 113820	1.6	3
31	Theoretical research on novel orthorhombic tungsten dinitride from first principles calculations.. <i>RSC Advances</i> , 2018 , 8, 9272-9276	3.7	3
30	Stable Structures and Superconductivity in a Y-Si System under High Pressure. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10388-10393	6.4	3
29	First principles study of LiAlO: new dense monoclinic phase under high pressure. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 115401	1.8	2
28	High-pressure modulated structures in beryllium chalcogenides. <i>Physical Review B</i> , 2019 , 100,	3.3	2
27	Novel high-pressure crystal structures of boron trifluoride. <i>Journal of Physics and Chemistry of Solids</i> , 2014 , 75, 1094-1098	3.9	2
26	Experimental clathrate superhydrides EuH6 and EuH9 at extreme pressure conditions. <i>Physical Review Research</i> , 2021 , 3,	3.9	2
25	Superconductive Sodium Carbides with Pentagon Carbon at High Pressures. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 5850-5856	6.4	2
24	Low-density superhard materials: computational study of Li-inserted B-substituted closo-carboranes LiBC11 and Li2B2C10. <i>RSC Advances</i> , 2016 , 6, 52695-52699	3.7	2
23	Novel high-pressure structure and superconductivity of titanium trisulfide. <i>Computational Materials Science</i> , 2019 , 158, 192-196	3.2	2
22	Pressure-induced structural modulations in coesite. <i>Physical Review B</i> , 2018 , 98,	3.3	2
21	Pressure-induced superconductivity and structure phase transition in Pt2HgSe3. <i>Npj Quantum Materials</i> , 2021 , 6,	5	2
20	Reply to Datchi et al.: Recovered phase CO2-V at low temperature and a newly predicted 3D-extended CO2 phase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E658-E659	11.5	1
19	Crystal Structures of CaBN at High Pressures. <i>Inorganic Chemistry</i> , 2017 , 56, 7449-7453	5.1	1
18	Metadynamics investigations of the AlN/GaN superlattice. <i>Europhysics Letters</i> , 2016 , 114, 46002	1.6	1
17	Novel boron channel-based structure of boron carbide at high pressures. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 455401	1.8	1
16	Oxysulfide Li2BeSO: A potential new material for solid electrolyte predicted from first principles. <i>Journal of Alloys and Compounds</i> , 2020 , 818, 152844	5.7	1

15	A new intermediate phase in compressed nitinol. <i>Journal of Alloys and Compounds</i> , 2020 , 817, 153234	5.7	1
14	Potassium-activated anionic copper and covalent Cu-Cu bonding in compressed K-Cu compounds. <i>Journal of Chemical Physics</i> , 2021 , 154, 134708	3.9	1
13	Retainable Superconductivity and Structural Transition in 1T-TaSe Under High Pressure. <i>Inorganic Chemistry</i> , 2021 , 60, 11385-11393	5.1	1
12	First-principles molecular dynamics simulations of single nitrogen bond structures in a N ₂ H ₂ system under pressure. <i>Solid State Communications</i> , 2019 , 290, 27-30	1.6	1
11	Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 21544-21553	3.6	1
10	Structure search of two-dimensional systems using CALYPSO methodology. <i>Frontiers of Physics</i> , 2022 , 17, 1	3.7	1
9	Computational prediction of a +4 oxidation state in Au via compressed AuO compound. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 015402	1.8	0
8	Phase transition and electronic properties of barium fluoride at high pressure. <i>Solid State Communications</i> , 2022 , 342, 114597	1.6	0
7	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. <i>Chemistry - A European Journal</i> , 2021 , 27, 17420-17427	4.8	0
6	Superconductivity in metal intercalated graphite-like boron-carbon-nitrogen. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021 , 402, 127348	2.3	0
5	Superconductive hydrogen-rich compounds under high pressure. <i>Applied Physics A: Materials Science and Processing</i> , 2021 , 127, 1	2.6	0
4	Low-Pressure Electrochemical Synthesis of Complex High-Pressure Superconducting Superhydrides.. <i>Physical Review Letters</i> , 2022 , 128, 186001	7.4	0
3	Anomalous optical and electronic properties of dense sodium. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010 , 374, 4458-4464	2.3	
2	Prediction of stable Cu structure and phase transition mechanism at ultra-high pressure: A comprehensive properties characterization by DFT calculation. <i>Physica B: Condensed Matter</i> , 2021 , 413538	2.8	
1	Structural characteristics and elasticities of coesite and coesite-II at high pressure. <i>New Journal of Physics</i> , 2020 , 22, 093044	2.9	