

Defang Duan

List of Publications by Year in Descending Order

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

135
papers

2,452
citations

24
h-index

43
g-index

144
ext. papers

3,228
ext. citations

4.4
avg, IF

4.99
L-index

#	Paper	IF	Citations
135	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure.. <i>Physical Review Letters</i> , 2022 , 128, 047001	7.4	8
134	Reply to the Comment on "High-temperature superconductivity in transition metallic hydrides MH (M = Mo, W, Nb, and Ta) under high pressure" by X. Zheng and J. Zheng, , 2022, , DOI: 10.1039/D1CP01474A.. <i>Physical Chemistry Chemical Physics</i> , 2022 , 24, 1898-1899	3.6	
133	A novel differential display material: KLuSiO: Tb/Bi phosphor with thermal response, time resolution and luminescence color for optical anti-counterfeiting. <i>Journal of Colloid and Interface Science</i> , 2022 , 608, 758-767	9.3	3
132	High T _c Superconductivity in Heavy Rare Earth Hydrides. <i>Chinese Physics Letters</i> , 2021 , 38, 107401	1.8	2
131	Proposed Superconducting Electride Li ₆ C by sp-Hybridized Cage States at Moderate Pressures. <i>Physical Review Letters</i> , 2021 , 127, 157002	7.4	1
130	Multistep Dissociation of Fluorine Molecules under Extreme Compression. <i>Physical Review Letters</i> , 2021 , 126, 225704	7.4	1
129	Synthesis of molecular metallic barium superhydride: pseudocubic BaH. <i>Nature Communications</i> , 2021 , 12, 273	17.4	29
128	Pressure-induced superconducting CSH with an HS framework. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22779-22784	3.6	4
127	CdS Induced Passivation toward High Efficiency and Stable Planar Perovskite Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 9771-9780	9.5	9
126	Pressure-Induced Superionicity of H in Hypervalent Sodium Silicon Hydrides. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7166-7172	6.4	0
125	First-principles investigation of rhodium hydrides under high pressure. <i>Physical Review B</i> , 2021 , 104,	3.3	1
124	Pressure-Induced Transition from Spin to Superconducting States in Novel MnN. <i>ACS Omega</i> , 2021 , 6, 21830-21836	3.9	
123	High-Temperature Superconducting Phases in Cerium Superhydride with a T _c up to 115K below a Pressure of 1 Megabar. <i>Physical Review Letters</i> , 2021 , 127, 117001	7.4	19
122	A novel hard superconductor obtained in di-molybdenum carbide (Mo ₂ C) with MoO ₆ octahedral structure. <i>Journal of Alloys and Compounds</i> , 2021 , 881, 160631	5.7	0
121	High-temperature superconductivity in transition metallic hydrides MH (M = Mo, W, Nb, and Ta) under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 6717-6724	3.6	6
120	Moderate Pressure Stabilized Pentazolene Cyclo-N Anion in Zn(N) Salt. <i>Inorganic Chemistry</i> , 2020 , 59, 8002-8012	5.1	15
119	Strain engineering induced indirect-direct band gap transition of difluorophosphorane. <i>Solid State Communications</i> , 2020 , 311, 113873	1.6	

118	Superconductivity of LaH ₁₀ and LaH ₁₆ polyhydrides. <i>Physical Review B</i> , 2020 , 101,	3.3	38
117	Superconducting praseodymium superhydrides. <i>Science Advances</i> , 2020 , 6, eaax6849	14.3	49
116	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2803-2811	16.4	28
115	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N ₆ anions. <i>Communications Chemistry</i> , 2020 , 3,	6.3	4
114	Ternary hypervalent silicon hydrides via lithium at high pressure. <i>Physical Review Materials</i> , 2020 , 4,	3.2	3
113	Superconducting Zirconium Polyhydrides at Moderate Pressures. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 646-651	6.4	12
112	Strain-engineering enables reversible semiconductor-metal transition of skutterudite IrAs ₃ . <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 1108-1114	6.8	1
111	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. <i>Physical Review Letters</i> , 2020 , 125, 217001	7.4	31
110	High-T _c state of lanthanum hydrides. <i>Physical Review B</i> , 2020 , 102,	3.3	3
109	Unexpected calcium polyhydride CaH: A possible route to dissociation of hydrogen molecules. <i>Journal of Chemical Physics</i> , 2019 , 150, 044507	3.9	10
108	Pressure-induced structures and properties in P ₈ compounds. <i>Solid State Communications</i> , 2019 , 293, 6-10	1.6	0
107	High-Pressure Bonding Mechanism of Selenium Nitrides. <i>Inorganic Chemistry</i> , 2019 , 58, 2397-2402	5.1	9
106	High-temperature superconductivity in sulfur hydride evidenced by alternating-current magnetic susceptibility. <i>National Science Review</i> , 2019 , 6, 713-718	10.8	32
105	Structural, Electronic, and Optical Properties of ZnO _{1-x} Te _x Alloys. <i>Physica Status Solidi - Rapid Research Letters</i> , 2019 , 13, 1900155	2.5	2
104	Metallic and anti-metallic properties of strongly covalently bonded energetic AlN nitrides. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 12029-12035	3.6	8
103	High-temperature superconductivity in ternary clathrate YCaH under high pressures. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 245404	1.8	10
102	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
101	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. <i>Inorganic Chemistry</i> , 2019 , 58, 2558-2564	5.1	12

100	Polyhydride CeH with an atomic-like hydrogen clathrate structure. <i>Nature Communications</i> , 2019 , 10, 3461	17.4	44
99	Nitrogen-rich GaN ₅ and GaN ₆ as high energy density materials with modest synthesis condition. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2019 , 383, 125859	2.3	7
98	Ternary superconducting cophosphorus hydrides stabilized via lithium. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	13
97	Role of TM-TM Connection Induced by Opposite d-Electron States on the Hardness of Transition-Metal (TM = Cr, W) Mononitrides. <i>Inorganic Chemistry</i> , 2019 , 58, 15573-15579	5.1	5
96	Structural and Dynamic Properties of the High-Pressure, High-Temperature Phase of Solid Ammonia Borane. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 6326-6332	3.8	4
95	First principle studies of ZnO _{1-x} S _x alloys under high pressure. <i>Journal of Alloys and Compounds</i> , 2019 , 788, 905-911	5.7	5
94	Structure and superconductivity of protactinium hydrides under high pressure. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 315403	1.8	4
93	Ab Initio Approach and Its Impact on Superconductivity. <i>Journal of Superconductivity and Novel Magnetism</i> , 2019 , 32, 53-60	1.5	16
92	Unusual structure and chemical behavior of potassium-indium under pressure. <i>Solid State Communications</i> , 2019 , 287, 77-82	1.6	2
91	The hardness mechanism and bonding properties of CrN ₂ : A first principle study. <i>Computational Materials Science</i> , 2019 , 158, 282-288	3.2	2
90	Revealing unusual rigid diamond net analogues in superhard titanium carbides.. <i>RSC Advances</i> , 2018 , 8, 14479-14487	3.7	4
89	High pressure structural stability of the Na-Te system. <i>AIP Advances</i> , 2018 , 8, 035123	1.5	
88	Emergent property of high hardness for C-rich ruthenium carbides: partial covalent Ru-Ru bonds. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 6108-6115	3.6	3
87	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. <i>Inorganic Chemistry</i> , 2018 , 57, 181-186	5.1	19
86	Insights into Antibonding Induced Energy Density Enhancement and Exotic Electronic Properties for Germanium Nitrides at Modest Pressures. <i>Inorganic Chemistry</i> , 2018 , 57, 10416-10423	5.1	2
85	Structures and properties of binary Mg Bi compounds under pressure. <i>Solid State Communications</i> , 2018 , 280, 18-23	1.6	3
84	First-principles study of ternary Li-Al-Te compounds under high pressure. <i>Solid State Communications</i> , 2018 , 270, 58-64	1.6	3
83	Pressure-Induced Stable Binary Compounds of Magnesium and Germanium. <i>Chemistry - A European Journal</i> , 2018 , 24, 18757-18761	4.8	1

82	Stable structures and superconductivity of an At-H system at high pressure. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 24783-24789	3.6	1
81	The Structure and Properties of Magnesium-Phosphorus Compounds Under Pressure. <i>Chemistry - A European Journal</i> , 2018 , 24, 11402-11406	4.8	5
80	High-pressure structures of helium and carbon dioxide from first-principles calculations. <i>Solid State Communications</i> , 2018 , 283, 9-13	1.6	2
79	Structure and superconductivity of hydrides at high pressures. <i>National Science Review</i> , 2017 , 4, 121-135	10.8	65
78	A Novel High-Density Phase and Amorphization of Nitrogen-Rich 1H-Tetrazole (CHN) under High Pressure. <i>Scientific Reports</i> , 2017 , 7, 39249	4.9	10
77	Alkaline-earth metal (Mg) polynitrides at high pressure as possible high-energy materials. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 9246-9252	3.6	43
76	A Novel Polymerization of Nitrogen in Beryllium Tetranitride at High Pressure. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 9766-9772	3.8	38
75	Bonding Properties of Aluminum Nitride at High Pressure. <i>Inorganic Chemistry</i> , 2017 , 56, 7494-7500	5.1	22
74	Stability of Sulfur Nitrides: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1515-1520	3.8	22
73	Divergent synthesis routes and superconductivity of ternary hydride MgSiH ₆ at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	32
72	Stability and Superconductivity of K-P Compounds under Pressure. <i>Inorganic Chemistry</i> , 2017 , 56, 12529-12534	12	12
71	Prediction of superconducting ternary hydride MgGeH: from divergent high-pressure formation routes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27406-27412	3.6	26
70	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. <i>Scientific Reports</i> , 2016 , 6, 18918	4.9	5
69	Strong covalent boron bonding induced extreme hardness of VB ₃ . <i>Journal of Alloys and Compounds</i> , 2016 , 688, 1101-1107	5.7	9
68	Ground state structures of tantalum tetraboride and triboride: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 18074-80	3.6	8
67	The stability of B ₆ octahedron in BaB ₆ under high pressure. <i>RSC Advances</i> , 2016 , 6, 18077-18081	3.7	7
66	Stability and properties of the Ru-H system at high pressure. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1516-20	3.6	20
65	High pressure structures and superconductivity of AlH ₃ (H ₂) predicted by first principles. <i>RSC Advances</i> , 2015 , 5, 5096-5101	3.7	26

64	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 22837-45	3.6	20
63	Structural, mechanical, and electronic properties of Rh ₂ B and RhB ₂ : first-principles calculations. <i>Scientific Reports</i> , 2015 , 5, 10500	4.9	10
62	Structures and Properties of Osmium Hydrides under Pressure from First Principle Calculation. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 15905-15911	3.8	25
61	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
60	Ab initio study of germanium-hydride compounds under high pressure. <i>RSC Advances</i> , 2015 , 5, 19432-19438	3.8	12
59	Structural properties of ammonium iodide under high pressure. <i>RSC Advances</i> , 2015 , 5, 40336-40340	3.7	7
58	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 13397-402	3.6	19
57	Cubic C96: a novel carbon allotrope with a porous nanocube network. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 10448-10452	13	38
56	Polymerization of Nitrogen in Ammonium Azide at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 25268-25272	3.8	14
55	Pressure-Induced Structures and Properties in Indium Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 9924-8	5.1	23
54	The hydrogen-bond effect on the high pressure behavior of hydrazinium monochloride. <i>Journal of Raman Spectroscopy</i> , 2015 , 46, 266-272	2.3	8
53	Ab initio study of native point defects in ZnO under pressure. <i>Solid State Communications</i> , 2015 , 201, 130-134	1.6	7
52	Optoelectronic investigation of corundum Mg ₄ Nb ₂ O ₉ single crystal. <i>Journal of Alloys and Compounds</i> , 2015 , 619, 240-243	5.7	3
51	Prediction of stoichiometric PoH _n compounds: crystal structures and properties. <i>RSC Advances</i> , 2015 , 5, 103445-103450	3.7	12
50	Pressure-induced decomposition of solid hydrogen sulfide. <i>Physical Review B</i> , 2015 , 91,	3.3	213
49	Ab initio investigation of CaO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2015 , 5, 11003	4.9	11
48	Ab initio structure determination of n-diamond. <i>Scientific Reports</i> , 2015 , 5, 13447	4.9	12
47	High-pressure polymorphism as a step towards high density structures of LiAlH ₄ . <i>Applied Physics Letters</i> , 2015 , 107, 041906	3.4	3

46	Pressure-induced structural changes in NH ₄ Br. <i>Journal of Chemical Physics</i> , 2015 , 143, 064505	3.9	1
45	Effects of magnetic ordering and electron correlations on the stability of FeN. <i>RSC Advances</i> , 2015 , 5, 31270-31274	3.7	13
44	Predicted structures and superconductivity of hypothetical Mg-CH ₄ compounds under high pressures. <i>Materials Research Express</i> , 2015 , 2, 046001	1.7	16
43	Enhancement of T _c in the atomic phase of iodine-doped hydrogen at high pressures. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 32335-40	3.6	13
42	Crystal structures and properties of nitrogen oxides under high pressure. <i>RSC Advances</i> , 2015 , 5, 103373-103379	3.7	10
41	Predicted Formation of H ₃ (+) in Solid Halogen Polyhydrides at High Pressures. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 11059-65	2.8	14
40	Ab initio study on the stability of N-doped ZnO under high pressure. <i>RSC Advances</i> , 2015 , 5, 16774-16779	3.7	2
39	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2014 , 4, 5759	4.9	19
38	Pressure-induced metallization of dense (H ₃)B ₂ with high-T _c superconductivity. <i>Scientific Reports</i> , 2014 , 4, 6968	4.9	502
37	Nitrogen concentration driving the hardness of rhenium nitrides. <i>Scientific Reports</i> , 2014 , 4, 4797	4.9	47
36	High-pressure close-packed structure of boron. <i>RSC Advances</i> , 2014 , 4, 203-207	3.7	17
35	Experimental verification of the high pressure crystal structures in NH ₃ BH ₃ . <i>Journal of Chemical Physics</i> , 2014 , 140, 244507	3.9	10
34	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. <i>RSC Advances</i> , 2014 , 4, 10133	3.7	52
33	Structural stability and compressive behavior of ZrH ₂ under hydrostatic pressure and nonhydrostatic pressure. <i>RSC Advances</i> , 2014 , 4, 46780-46786	3.7	11
32	High pressure superconducting phase of BI ₃ : an ab initio study. <i>RSC Advances</i> , 2014 , 4, 32068-32074	3.7	3
31	p-Aminobenzoic acid polymorphs under high pressures. <i>RSC Advances</i> , 2014 , 4, 15534-15541	3.7	21
30	Modulated T carbon-like carbon allotropes: an ab initio study. <i>RSC Advances</i> , 2014 , 4, 17364	3.7	28
29	Crystal structures and properties of the CH ₄ H ₂ compound under high pressure. <i>RSC Advances</i> , 2014 , 4, 37569	3.7	6

28	Ultrahard boron-rich tantalum boride: Monoclinic TaB 4. <i>Journal of Alloys and Compounds</i> , 2014 , 617, 660-664	5.7	16
27	Hydrogen Bond in Compressed Solid Hydrazine. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 3236-3243	3.8	14
26	Pressure-Induced Diversity of π -Stacking Motifs and Amorphous Polymerization in Pyrrole. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 12420-12427	3.8	12
25	Optical floating zone method growth and optical properties of corundum Mg ₄ Nb ₂ O ₉ single crystal. <i>Journal of Crystal Growth</i> , 2014 , 402, 109-112	1.6	3
24	Pressure induced phase transition in MH ₂ (M = V, Nb). <i>Journal of Chemical Physics</i> , 2014 , 140, 114703	3.9	16
23	The crystal structure of IrB ₂ : a first-principle calculation. <i>RSC Advances</i> , 2014 , 4, 63442-63446	3.7	10
22	The structure and dynamics analysis of one-dimension confined C _{3V} symmetrical C ₆₀ H ₁₈ molecules in single-wall carbon nanotube. <i>CrystEngComm</i> , 2013 , 15, 7723	3.3	5
21	Structure determination of ultra dense magnesium borohydride: a first-principles study. <i>Journal of Chemical Physics</i> , 2013 , 138, 214503	3.9	3
20	Structural and Electronic Changes of SnBr ₄ under High Pressure. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 8381-8387	3.8	7
19	Pressure-Driven Topological Transformations of Iodine Confined in One-Dimensional Channels. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 25052-25058	3.8	19
18	Predicted novel metallic metastable phases of polymeric nitrogen at high pressures. <i>New Journal of Physics</i> , 2013 , 15, 013010	2.9	13
17	How to get superhard MnB ₂ : a first-principles study. <i>Journal of Materials Chemistry</i> , 2012 , 22, 17630		8
16	Elastic properties study of single crystal NH ₃ up to 26 GPa. <i>Journal of Raman Spectroscopy</i> , 2012 , 43, 526-531	2.3	6
15	Superconductive superhard phase of BC ₇ : Predicted via ab initio calculations. <i>Diamond and Related Materials</i> , 2011 , 20, 454-457	3.5	6
14	Structural properties and halogen bonds of cyanuric chloride under high pressure. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4639-44	3.4	20
13	Structural transitions of NaAlH ₄ under high pressure by first-principles calculations. <i>Physica B: Condensed Matter</i> , 2011 , 406, 1612-1614	2.8	4
12	Hydrogen bond symmetrization and superconducting phase of HBr and HCl under high pressure: An ab initio study. <i>Journal of Chemical Physics</i> , 2010 , 133, 074509	3.9	37
11	A new high-pressure polar phase of crystalline bromoform: a first-principles study. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 13933-9	3.4	6

10	Pressure-induced phase transition in hydrogen-bonded supramolecular structure: guanidinium nitrate. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 6765-9	3.4	30
9	New high-pressure phase of BaHf ₂ predicted by ab initio studies. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 225401	1.8	5
8	The crystal structure and superconducting properties of monatomic bromine. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 015702	1.8	9
7	Effect of nonhydrostatic pressure on superconductivity of monatomic iodine: An ab initio study. <i>Physical Review B</i> , 2009 , 79,	3.3	20
6	Stability of hydrogen-bonded supramolecular architecture under high pressure conditions: pressure-induced amorphization in melamine-boric acid adduct. <i>Langmuir</i> , 2009 , 25, 4787-91	4	46
5	Pressure-induced phase transition in hydrogen-bonded supramolecular adduct formed by cyanuric acid and melamine. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 14719-24	3.4	49
4	Near-edge X-ray absorption fine structure of solid oxygen under high pressure: A density functional theory study. <i>Solid State Communications</i> , 2008 , 147, 126-129	1.6	5
3	Ab Initio Investigation on the Doped H ₃ S by V, VI, and VII Group Elements Under High Pressure. <i>Journal of Superconductivity and Novel Magnetism</i> , 1	1.5	1
2	Retainable Bandgap Narrowing and Enhanced Photoluminescence in Mn-Doped and Undoped Cs ₂ NaBiCl ₆ Double Perovskites by Pressure Engineering. <i>Advanced Optical Materials</i> , 2101892	8.1	4
1	New Cage-Like Cerium Trihydride Stabilized at Ambient Conditions. <i>CCS Chemistry</i> , 1012-1018	7.2	1