Defang Duan

List of Publications by Citations

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	Pressure-induced metallization of dense (H_2S)H_2 with high-Tc superconductivity. *Scientific Reports*, **2014**, 4, 6968	4.9	502
134	Pressure-induced decomposition of solid hydrogen sulfide. *Physical Review B*, **2015**, 91,	3.3	213
133	Structure and superconductivity of hydrides at high pressures. *National Science Review*, **2017**, 4, 121-135	10.8	65
132	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. *RSC Advances*, **2014**, 4, 10133	3.7	52
131	Superconducting praseodymium superhydrides. *Science Advances*, **2020**, 6, eaax6849	14.3	49
130	Pressure-induced phase transition in hydrogen-bonded supramolecular adduct formed by cyanuric acid and melamine. *Journal of Physical Chemistry B*, **2009**, 113, 14719-24	3.4	49
129	Nitrogen concentration driving the hardness of rhenium nitrides. *Scientific Reports*, **2014**, 4, 4797	4.9	47
128	Stability of hydrogen-bonded supramolecular architecture under high pressure conditions: pressure-induced amorphization in melamine-boric acid adduct. *Langmuir*, **2009**, 25, 4787-91	4	46
127	Polyhydride CeH with an atomic-like hydrogen clathrate structure. *Nature Communications*, **2019**, 10, 3461	17.4	44
126	Alkaline-earth metal (Mg) polynitrides at high pressure as possible high-energy materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 9246-9252	3.6	43
125	A Novel Polymerization of Nitrogen in Beryllium Tetranitride at High Pressure. *Journal of Physical Chemistry C*, **2017**, 121, 9766-9772	3.8	38
124	Cubic C96: a novel carbon allotrope with a porous nanocube network. *Journal of Materials Chemistry A*, **2015**, 3, 10448-10452	13	38
123	Superconductivity of LaH10 and LaH16 polyhydrides. *Physical Review B*, **2020**, 101,	3.3	38
122	Hydrogen bond symmetrization and superconducting phase of HBr and HCl under high pressure: An ab initio study. *Journal of Chemical Physics*, **2010**, 133, 074509	3.9	37
121	Divergent synthesis routes and superconductivity of ternary hydride MgSiH6 at high pressure. *Physical Review B*, **2017**, 96,	3.3	32
120	High-temperature superconductivity in sulfur hydride evidenced by alternating-current magnetic susceptibility. *National Science Review*, **2019**, 6, 713-718	10.8	32
119	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. *Physical Review Letters*, **2020**, 125, 217001	7.4	31

118	Pressure-induced phase transition in hydrogen-bonded supramolecular structure: guanidinium nitrate. *Journal of Physical Chemistry B*, **2010**, 114, 6765-9	3.4	30
117	Synthesis of molecular metallic barium superhydride: pseudocubic BaH. *Nature Communications*, **2021**, 12, 273	17.4	29
116	High-Pressure Synthesis of Magnetic Neodymium Polyhydrides. *Journal of the American Chemical Society*, **2020**, 142, 2803-2811	16.4	28
115	Modulated T carbon-like carbon allotropes: an ab initio study. *RSC Advances*, **2014**, 4, 17364	3.7	28
114	High pressure structures and superconductivity of AlH3(H2) predicted by first principles. *RSC Advances*, **2015**, 5, 5096-5101	3.7	26
113	Prediction of superconducting ternary hydride MgGeH: from divergent high-pressure formation routes. *Physical Chemistry Chemical Physics*, **2017**, 19, 27406-27412	3.6	26
112	Structures and Properties of Osmium Hydrides under Pressure from First Principle Calculation. *Journal of Physical Chemistry C*, **2015**, 119, 15905-15911	3.8	25
111	Pressure-Induced Structures and Properties in Indium Hydrides. *Inorganic Chemistry*, **2015**, 54, 9924-8	5.1	23
110	Bonding Properties of Aluminum Nitride at High Pressure. *Inorganic Chemistry*, **2017**, 56, 7494-7500	5.1	22
109	Stability of Sulfur Nitrides: A First-Principles Study. *Journal of Physical Chemistry C*, **2017**, 121, 1515-1520	3.8	22
108	p-Aminobenzoic acid polymorphs under high pressures. *RSC Advances*, **2014**, 4, 15534-15541	3.7	21
107	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. *Physical Chemistry Chemical Physics*, **2015**, 17, 22837-45	3.6	20
106	Stability and properties of the Ru-H system at high pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 1516-20	3.6	20
105	Structural properties and halogen bonds of cyanuric chloride under high pressure. *Journal of Physical Chemistry B*, **2011**, 115, 4639-44	3.4	20
104	Effect of nonhydrostatic pressure on superconductivity of monatomic iodine: An ab initio study. *Physical Review B*, **2009**, 79,	3.3	20
103	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. *Scientific Reports*, **2014**, 4, 5759	4.9	19
102	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 13397-402	3.6	19
101	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. *Inorganic Chemistry*, **2018**, 57, 181-186	5.1	19

100	Pressure-Driven Topological Transformations of Iodine Confined in One-Dimensional Channels. *Journal of Physical Chemistry C*, **2013**, 117, 25052-25058	3.8	19
99	High-Temperature Superconducting Phases in Cerium Superhydride with a T_{c} up to 115 K below a Pressure of 1 Megabar. *Physical Review Letters*, **2021**, 127, 117001	7.4	19
98	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. *Scientific Reports*, **2015**, 5, 11381	4.9	18
97	High-pressure close-packed structure of boron. *RSC Advances*, **2014**, 4, 203-207	3.7	17
96	Ultrahard boron-rich tantalum boride: Monoclinic TaB 4. *Journal of Alloys and Compounds*, **2014**, 617, 660-664	5.7	16
95	Predicted structures and superconductivity of hypothetical Mg-CH4compounds under high pressures. *Materials Research Express*, **2015**, 2, 046001	1.7	16
94	Pressure induced phase transition in MH (M = V, Nb). *Journal of Chemical Physics*, **2014**, 140, 114703	3.9	16
93	Ab Initio Approach and Its Impact on Superconductivity. *Journal of Superconductivity and Novel Magnetism*, **2019**, 32, 53-60	1.5	16
92	Moderate Pressure Stabilized Pentazolate Cyclo-N Anion in Zn(N) Salt. *Inorganic Chemistry*, **2020**, 59, 8002-8012	5.1	15
91	Polymerization of Nitrogen in Ammonium Azide at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 25268-25272	3.8	14
90	Hydrogen Bond in Compressed Solid Hydrazine. *Journal of Physical Chemistry C*, **2014**, 118, 3236-3243	3.8	14
89	Predicted Formation of H3(+) in Solid Halogen Polyhydrides at High Pressures. *Journal of Physical Chemistry A*, **2015**, 119, 11059-65	2.8	14
88	Ternary superconducting cophosphorus hydrides stabilized via lithium. *Npj Computational Materials* , **2019**, 5,	10.9	13
87	Effects of magnetic ordering and electron correlations on the stability of FeN. *RSC Advances*, **2015**, 5, 31270-31274	3.7	13
86	Enhancement of T(c) in the atomic phase of iodine-doped hydrogen at high pressures. *Physical Chemistry Chemical Physics*, **2015**, 17, 32335-40	3.6	13
85	Predicted novel metallic metastable phases of polymeric nitrogen at high pressures. *New Journal of Physics*, **2013**, 15, 013010	2.9	13
84	Stability and Superconductivity of K-P Compounds under Pressure. *Inorganic Chemistry*, **2017**, 56, 12529-12534	5.1	12
83	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. *Inorganic Chemistry*, **2019**, 58, 2558-2564	5.1	12

82	Ab initio study of germanium-hydride compounds under high pressure. *RSC Advances*, **2015**, 5, 19432-19438	3.7	12
81	Pressure-Induced Diversity of Stacking Motifs and Amorphous Polymerization in Pyrrole. *Journal of Physical Chemistry C*, **2014**, 118, 12420-12427	3.8	12
80	Prediction of stoichiometric PoHn compounds: crystal structures and properties. *RSC Advances*, **2015**, 5, 103445-103450	3.7	12
79	Ab initio structure determination of n-diamond. *Scientific Reports*, **2015**, 5, 13447	4.9	12
78	Superconducting Zirconium Polyhydrides at Moderate Pressures. *Journal of Physical Chemistry Letters*, **2020**, 11, 646-651	6.4	12
77	Structural stability and compressive behavior of ZrH2 under hydrostatic pressure and nonhydrostatic pressure. *RSC Advances*, **2014**, 4, 46780-46786	3.7	11
76	Ab initio investigation of CaO-ZnO alloys under high pressure. *Scientific Reports*, **2015**, 5, 11003	4.9	11
75	A Novel High-Density Phase and Amorphization of Nitrogen-Rich 1H-Tetrazole (CHN) under High Pressure. *Scientific Reports*, **2017**, 7, 39249	4.9	10
74	Unexpected calcium polyhydride CaH: A possible route to dissociation of hydrogen molecules. *Journal of Chemical Physics*, **2019**, 150, 044507	3.9	10
73	High-temperature superconductivity in ternary clathrate YCaH under high pressures. *Journal of Physics Condensed Matter*, **2019**, 31, 245404	1.8	10
72	Structural, mechanical, and electronic properties of Rh2B and RhB2: first-principles calculations. *Scientific Reports*, **2015**, 5, 10500	4.9	10
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62	How to get superhard MnB2: a first-principles study. *Journal of Materials Chemistry*, **2012**, 22, 17630		8
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60	Structural properties of ammonium iodide under high pressure. *RSC Advances*, **2015**, 5, 40336-40340	3.7	7
59	Ab initio study of native point defects in ZnO under pressure. *Solid State Communications*, **2015**, 201, 130-134	1.6	7
58	The stability of B6 octahedron in BaB6 under high pressure. *RSC Advances*, **2016**, 6, 18077-18081	3.7	7
57	Nitrogen-rich GaN5 and GaN6 as high energy density materials with modest synthesis condition. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 125859	2.3	7
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55	Crystal structures and properties of the CH4H2 compound under high pressure. *RSC Advances*, **2014** , 4, 37569	3.7	6
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53	Superconductive superhard phase of BC7: Predicted via ab initio calculations. *Diamond and Related Materials*, **2011**, 20, 454-457	3.5	6
52	A new high-pressure polar phase of crystalline bromoform: a first-principles study. *Journal of Physical Chemistry B*, **2010**, 114, 13933-9	3.4	6
51	High-temperature superconductivity in transition metallic hydrides MH (M = Mo, W, Nb, and Ta) under high pressure. *Physical Chemistry Chemical Physics*, **2021**, 23, 6717-6724	3.6	6
50	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. *Scientific Reports*, **2016**, 6, 18918	4.9	5
49	Role of TM-TM Connection Induced by Opposite d-Electron States on the Hardness of Transition-Metal (TM = Cr, W) Mononitrides. *Inorganic Chemistry*, **2019**, 58, 15573-15579	5.1	5
48	The structure and dynamics analysis of one-dimension confined C3V symmetrical C60H18 molecules in single-wall carbon nanotube. *CrystEngComm*, **2013**, 15, 7723	3.3	5
47	New high-pressure phase of BaH predicted by ab initio studies. *Journal of Physics Condensed Matter*, **2010**, 22, 225401	1.8	5

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39	Structural and Dynamic Properties of the High-Pressure, High-Temperature Phase of Solid Ammonia Borane. *Journal of Physical Chemistry C*, **2019**, 123, 6326-6332	3.8	4
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35	Optoelectronic investigation of corundum Mg4Nb2O9 single crystal. *Journal of Alloys and Compounds*, **2015**, 619, 240-243	5.7	3
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15	Ab Initio Investigation on the Doped H3S by V, VI, and VII Group Elements Under High Pressure. *Journal of Superconductivity and Novel Magnetism*,1	1.5	1
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13	Strain-engineering enables reversible semiconductor□metal transition of skutterudite IrAs3. *Inorganic Chemistry Frontiers*, **2020**, 7, 1108-1114	6.8	1
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4	Strain engineering induced indirect-direct band gap transition of difluorphosphorane. *Solid State Communications*, **2020**, 311, 113873	1.6	
3	High pressure structural stability of the Na-Te system. *AIP Advances*, **2018**, 8, 035123	1.5	
2	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.. *Physical Chemistry Chemical Physics*, **2022**, 24, 1898-1899	3.6	
1	Pressure-Induced Transition from Spin to Superconducting States in Novel MnN. *ACS Omega*, **2021**, 6, 21830-21836	3.9	