Da Li

List of Publications by Citations

96	1,818	19	40
papers	citations	h-index	g-index

106	2,340	4.2	4.64
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
96	Pressure-induced metallization of dense (H2S)H2 with high-Tc superconductivity. *Scientific Reports*, **2014**, 4, 6968	4.9	502
95	Pressure-induced decomposition of solid hydrogen sulfide. *Physical Review B*, **2015**, 91,	3.3	213
94	Lowest enthalpy polymorph of cold-compressed graphite phase. *Physical Chemistry Chemical Physics*, **2012**, 14, 4347-50	3.6	77
93	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. *RSC Advances*, **2014**, 4, 10133	3.7	52
92	Nitrogen concentration driving the hardness of rhenium nitrides. *Scientific Reports*, **2014**, 4, 4797	4.9	47
91	Alkaline-earth metal (Mg) polynitrides at high pressure as possible high-energy materials. *Physical Chemistry Chemical Physics*, **2017**, 19, 9246-9252	3.6	43
90	A Novel Polymerization of Nitrogen in Beryllium Tetranitride at High Pressure. *Journal of Physical Chemistry C*, **2017**, 121, 9766-9772	3.8	38
89	Cubic C96: a novel carbon allotrope with a porous nanocube network. *Journal of Materials Chemistry A*, **2015**, 3, 10448-10452	13	38
88	Cubic gauche-CN: A superhard metallic compound predicted via first-principles calculations. *Journal of Chemical Physics*, **2010**, 133, 044512	3.9	34
87	Divergent synthesis routes and superconductivity of ternary hydride MgSiH6 at high pressure. *Physical Review B*, **2017**, 96,	3.3	32
86	Large Volume Collapse during Pressure-Induced Phase Transition in Lithium Amide. *Journal of Physical Chemistry C*, **2012**, 116, 9744-9749	3.8	29
85	Modulated T carbon-like carbon allotropes: an ab initio study. *RSC Advances*, **2014**, 4, 17364	3.7	28
84	High pressure structures and superconductivity of AlH3(H2) predicted by first principles. *RSC Advances*, **2015**, 5, 5096-5101	3.7	26
83	Prediction of superconducting ternary hydride MgGeH: from divergent high-pressure formation routes. *Physical Chemistry Chemical Physics*, **2017**, 19, 27406-27412	3.6	26
82	Structures and Properties of Osmium Hydrides under Pressure from First Principle Calculation. *Journal of Physical Chemistry C*, **2015**, 119, 15905-15911	3.8	25
81	Pressure-Induced Structures and Properties in Indium Hydrides. *Inorganic Chemistry*, **2015**, 54, 9924-8	5.1	23
80	Bonding Properties of Aluminum Nitride at High Pressure. *Inorganic Chemistry*, **2017**, 56, 7494-7500	5.1	22

79	Stability of Sulfur Nitrides: A First-Principles Study. *Journal of Physical Chemistry C*, **2017**, 121, 1515-1520	3.8	22
78	Stability and properties of the Ru-H system at high pressure. *Physical Chemistry Chemical Physics*, **2016**, 18, 1516-20	3.6	20
77	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. *Scientific Reports*, **2014**, 4, 5759	4.9	19
76	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. *Inorganic Chemistry*, **2018**, 57, 181-186	5.1	19
75	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. *Scientific Reports*, **2015**, 5, 11381	4.9	18
74	High-temperature superconductivity in compressed solid silane. *Scientific Reports*, **2015**, 5, 8845	4.9	18
73	High-pressure close-packed structure of boron. *RSC Advances*, **2014**, 4, 203-207	3.7	17
72	Pressure-induced superconducting ternary hydride H3SXe: A theoretical investigation. *Frontiers of Physics*, **2018**, 13, 1	3.7	16
71	Ultrahard boron-rich tantalum boride: Monoclinic TaB 4. *Journal of Alloys and Compounds*, **2014**, 617, 660-664	5.7	16
70	Predicted structures and superconductivity of hypothetical Mg-CH4compounds under high pressures. *Materials Research Express*, **2015**, 2, 046001	1.7	16
69	Moderate Pressure Stabilized Pentazolate Cyclo-N Anion in Zn(N) Salt. *Inorganic Chemistry*, **2020**, 59, 8002-8012	5.1	15
68	Polymerization of Nitrogen in Ammonium Azide at High Pressures. *Journal of Physical Chemistry C*, **2015**, 119, 25268-25272	3.8	14
67	Predicted Formation of H3(+) in Solid Halogen Polyhydrides at High Pressures. *Journal of Physical Chemistry A*, **2015**, 119, 11059-65	2.8	14
66	Investigation of stable germane structures under high-pressure. *Physical Chemistry Chemical Physics* , **2015**, 17, 27630-5	3.6	13
65	Ternary superconducting cophosphorus hydrides stabilized via lithium. *Npj Computational Materials* , **2019**, 5,	10.9	13
64	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
63	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. *Inorganic Chemistry*, **2019**, 58, 2558-2564	5.1	12
62	Ab initio study of germanium-hydride compounds under high pressure. *RSC Advances*, **2015**, 5, 19432-19438	3.7	12

61	Prediction of stoichiometric PoHn compounds: crystal structures and properties. *RSC Advances*, **2015**, 5, 103445-103450	3.7	12
60	Ab initio structure determination of n-diamond. *Scientific Reports*, **2015**, 5, 13447	4.9	12
59	Ab initio investigation of CaO-ZnO alloys under high pressure. *Scientific Reports*, **2015**, 5, 11003	4.9	11
58	High-temperature superconductivity in ternary clathrate YCaH under high pressures. *Journal of Physics Condensed Matter*, **2019**, 31, 245404	1.8	10
57	Structural, mechanical, and electronic properties of Rh2B and RhB2: first-principles calculations. *Scientific Reports*, **2015**, 5, 10500	4.9	10
56	The crystal structure of IrB2: a first-principle calculation. *RSC Advances*, **2014**, 4, 63442-63446	3.7	10
55	Local Carbon Concentration Determines the Graphene Edge Structure. *Journal of Physical Chemistry Letters*, **2020**, 11, 3451-3457	6.4	10
54	High-Pressure Bonding Mechanism of Selenium Nitrides. *Inorganic Chemistry*, **2019**, 58, 2397-2402	5.1	9
53	Strong covalent boron bonding induced extreme hardness of VB3. *Journal of Alloys and Compounds*, **2016**, 688, 1101-1107	5.7	9
52	Environment-dependent edge reconstruction of transition metal dichalcogenides: a global search. *Materials Today Advances*, **2020**, 8, 100079	7.4	9
51	Metallic and anti-metallic properties of strongly covalently bonded energetic AlN nitrides. *Physical Chemistry Chemical Physics*, **2019**, 21, 12029-12035	3.6	8
50	Ground state structures of tantalum tetraboride and triboride: an ab initio study. *Physical Chemistry Chemical Physics*, **2016**, 18, 18074-80	3.6	8
49	Ab initio study of native point defects in ZnO under pressure. *Solid State Communications*, **2015**, 201, 130-134	1.6	7
48	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
47	Ab initio studies of copper hydrides under high pressure. *Frontiers of Physics*, **2019**, 14, 1	3.7	6
46	Structural phase transition and bonding properties of high-pressure polymeric CaN3. *RSC Advances*, **2018**, 8, 4314-4320	3.7	6
45	Pressure-induced phase transition of SnH4: a new layered structure. *RSC Advances*, **2016**, 6, 10456-10461	3.7	6
44	Crystal structures and properties of the CH4H2 compound under high pressure. *RSC Advances*, **2014**, 4, 37569	3.7	6

43	A novel stable hydrogen-rich SnH8 under high pressure. *RSC Advances*, **2015**, 5, 107637-107641	3.7	6
42	Pressure-stabilized polymerization of nitrogen in alkaline-earth-metal strontium nitrides. *Physical Chemistry Chemical Physics*, **2020**, 22, 5242-5248	3.6	6
41	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. *Scientific Reports*, **2016**, 6, 18918	4.9	5
40	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
39	Anisotropic Angstrom-Wide Conductive Channels in Black Phosphorus by Top-down Cu Intercalation. *Nano Letters*, **2021**, 21, 6336-6342	11.5	5
38	First principle studies of ZnO1-xSx alloys under high pressure. *Journal of Alloys and Compounds*, **2019**, 788, 905-911	5.7	5
37	Pressure-Induced Amorphization and Recrystallization of SnI2. *Journal of Physical Chemistry C*, **2015** , 119, 19312-19317	3.8	4
36	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N6 anions. *Communications Chemistry*, **2020**, 3,	6.3	4
35	Revealing unusual rigid diamond net analogues in superhard titanium carbides.. *RSC Advances*, **2018** , 8, 14479-14487	3.7	4
34	High-pressure phase transition of MH□(M: Er, Ho). *Journal of Chemical Physics*, **2014**, 141, 054703	3.9	4
33	Formation of twelve-fold iodine coordination at high pressure.. *Nature Communications*, **2022**, 13, 412	17.4	4
32	Pressure-induced structural transformation of CaC2. *Journal of Chemical Physics*, **2016**, 144, 194506	3.9	4
31	Structure and superconductivity of protactinium hydrides under high pressure. *Journal of Physics Condensed Matter*, **2019**, 31, 315403	1.8	4
30	Edge reconstructions of black phosphorene: a global search. *Nanoscale*, **2021**, 13, 4085-4091	7.7	4
29	Structural and electrical properties of Ga□e systems under high pressure. *Chinese Physics B*, **2019**, 28, 056104	1.2	3
28	Emergent property of high hardness for C-rich ruthenium carbides: partial covalent Ru-Ru bonds. *Physical Chemistry Chemical Physics*, **2018**, 20, 6108-6115	3.6	3
27	High pressure superconducting phase of BI3: an ab initio study. *RSC Advances*, **2014**, 4, 32068-32074	3.7	3
26	Synthesis and characterization of a strong ferromagnetic and high hardness intermetallic compound FeB. *Physical Chemistry Chemical Physics*, **2020**, 22, 27425-27432	3.6	3

25	Two-dimensional C5678: a promising carbon-based high-performance lithium-ion battery anode. *Materials Advances*, **2021**, 2, 398-402	3.3	3
24	Stability of hydrogen-terminated graphene edges. *Physical Chemistry Chemical Physics*, **2021**, 23, 13261-13266	3.3	3
23	First-principles study of ternary Li-Al-Te compounds under high pressure. *Solid State Communications*, **2018**, 270, 58-64	1.6	3
22	Structural, Electronic, and Optical Properties of ZnO1 □xTex Alloys. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1900155	2.5	2
21	Ground State Structures of Boron-Rich Rhodium Boride: An Ab Initio Study. *Chinese Physics Letters*, **2018**, 35, 016401	1.8	2
20	Insights into Antibonding Induced Energy Density Enhancement and Exotic Electronic Properties for Germanium Nitrides at Modest Pressures. *Inorganic Chemistry*, **2018**, 57, 10416-10423	5.1	2
19	A theoretical investigation on phase transition and dissociation of ammonium bromide under high pressure. *Science Bulletin*, **2014**, 59, 5272-5277		2
18	Crystal structures and properties of nitrogen oxides under high pressure. *RSC Advances*, **2015**, 5, 103373-103379	3.7	2
17	Ab initio study on the stability of N-doped ZnO under high pressure. *RSC Advances*, **2015**, 5, 16774-16779	3.7	2
16	Ab initio studies on ammonium iodine under high pressure. *Chinese Physics B*, **2020**, 29, 053104	1.2	2
15	Two-dimensional few-layered Janus diamond nanofilms with boron-terminated surfaces: First-principles calculation. *Thin Solid Films*, **2021**, 722, 138570	2.2	2
14	Unraveling electrochemical CO reduction of the single-atom transition metals supported on N-doped phosphorene. *Applied Surface Science*, **2021**, 545, 148953	6.7	2
13	Carbon and Oxygen Coordinating Atoms Adjust Transition Metal Single-Atom Catalysts Based On Boron Nitride Monolayers for Highly Efficient CO Electroreduction. *ACS Applied Materials & Interfaces*, **2021**, 13, 18934-18943	9.5	2
12	The hardness mechanism and bonding properties of CrN2: A first principle study. *Computational Materials Science*, **2019**, 158, 282-288	3.2	2
11	Defects of monolayer PbI: a computational study. *Physical Chemistry Chemical Physics*, **2021**, 23, 20553-20559	3.3	2
10	Structural and Electrical Properties of Be x Zn1□ O Alloys under High Pressure. *Chinese Physics Letters*, **2021**, 38, 026101	1.8	2
9	High-pressure structures of helium and carbon dioxide from first-principles calculations. *Solid State Communications*, **2018**, 283, 9-13	1.6	2
8	High-pressure formation of antimony nitrides: a first-principles study.. *RSC Advances*, **2020**, 10, 2448-2453	3.7	1

7	Proposed Superconducting Electride Li_{6}C by sp-Hybridized Cage States at Moderate Pressures. *Physical Review Letters*, **2021**, 127, 157002	7.4	1
6	Strain-engineering enables reversible semiconductor□metal transition of skutterudite IrAs3. *Inorganic Chemistry Frontiers*, **2020**, 7, 1108-1114	6.8	1
5	Stable structures and superconductivity of an At-H system at high pressure. *Physical Chemistry Chemical Physics*, **2018**, 20, 24783-24789	3.6	1
4	Correlations of Ionic Migration and Deep-Level Traps Leads to Surface Defect Formation in Perovskite Solar Cells. *Journal of Physical Chemistry C*, **2021**, 125, 19551-19559	3.8	1
3	First-principle studies on the Li□Te system. *Materials Research Express*, **2017**, 4, 015701	1.7	
2	Strain engineering induced indirect-direct band gap transition of difluorphosphorane. *Solid State Communications*, **2020**, 311, 113873	1.6	
1	High pressure structural stability of the Na-Te system. *AIP Advances*, **2018**, 8, 035123	1.5	