Da Li

List of Publications by Year
in descending order

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99 papers	2,800 citations	236612 25 h-index	197535 49 g-index
106 all docs	106 docs citations	106 times ranked	1645 citing authors

#	Article	IF	Citations
1	Pressure-induced metallization of dense (H2S)2H2 with high-Tc superconductivity. Scientific Reports, 2014, 4, 6968.	1.6	802
2	Pressure-induced decomposition of solid hydrogen sulfide. Physical Review B, 2015, 91, .	1.1	255
3	Lowest enthalpy polymorph of cold-compressed graphite phase. Physical Chemistry Chemical Physics, 2012, 14, 4347.	1.3	80
4	Alkaline-earth metal (Mg) polynitrides at high pressure as possible high-energy materials. Physical Chemistry Chemical Physics, 2017, 19, 9246-9252.	1.3	77
5	A Novel Polymerization of Nitrogen in Beryllium Tetranitride at High Pressure. Journal of Physical Chemistry C, 2017, 121, 9766-9772.	1.5	67
6	Nitrogen concentration driving the hardness of rhenium nitrides. Scientific Reports, 2014, 4, 4797.	1.6	61
7	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
8	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. RSC Advances, 2014, 4, 10133.	1.7	55
9	Cubic C₉₆: a novel carbon allotrope with a porous nanocube network. Journal of Materials Chemistry A, 2015, 3, 10448-10452.	5.2	47
10	Cubic gauche-CN: A superhard metallic compound predicted via first-principles calculations. Journal of Chemical Physics, 2010, 133, 044512.	1.2	40
11	Prediction of superconducting ternary hydride MgGeH₆: from divergent high-pressure formation routes. Physical Chemistry Chemical Physics, 2017, 19, 27406-27412.	1.3	40
12	Ternary superconducting cophosphorus hydrides stabilized via lithium. Npj Computational Materials, 2019, 5, .	3.5	38
13	Pressure-Induced Structures and Properties in Indium Hydrides. Inorganic Chemistry, 2015, 54, 9924-9928.	1.9	34
14	Bonding Properties of Aluminum Nitride at High Pressure. Inorganic Chemistry, 2017, 56, 7494-7500.	1.9	34
15	High pressure structures and superconductivity of AlH₃(H₂) predicted by first principles. RSC Advances, 2015, 5, 5096-5101.	1.7	33
16	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. Inorganic Chemistry, 2019, 58, 2558-2564.	1.9	33
17	Large Volume Collapse during Pressure-Induced Phase Transition in Lithium Amide. Journal of Physical Chemistry C, 2012, 116, 9744-9749.	1.5	32
18	High-temperature superconductivity in ternary clathrate YCaH₁₂ under high pressures. Journal of Physics Condensed Matter, 2019, 31, 245404.	0.7	31

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19	Moderate Pressure Stabilized Pentazolate Cyclo-N₅^{â€“} Anion in Zn(N₅)₂ Salt. Inorganic Chemistry, 2020, 59, 8002-8012.	1.9	31
20	Stability of Sulfur Nitrides: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 1515-1520.	1.5	30
21	Modulated T carbon-like carbon allotropes: an ab initio study. RSC Advances, 2014, 4, 17364.	1.7	29
22	Structures and Properties of Osmium Hydrides under Pressure from First Principle Calculation. Journal of Physical Chemistry C, 2015, 119, 15905-15911.	1.5	29
23	Pressure-induced superconducting ternary hydride H3SXe: A theoretical investigation. Frontiers of Physics, 2018, 13, 1.	2.4	29
24	Ultrahard boron-rich tantalum boride: Monoclinic TaB 4. Journal of Alloys and Compounds, 2014, 617, 660-664.	2.8	28
25	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. Scientific Reports, 2014, 4, 5759.	1.6	26
26	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. Scientific Reports, 2015, 5, 11381.	1.6	26
27	Stability and properties of the Ruâ€“H system at high pressure. Physical Chemistry Chemical Physics, 2016, 18, 1516-1520.	1.3	26
28	High-temperature Superconductivity in compressed Solid Silane. Scientific Reports, 2015, 5, 8845.	1.6	25
29	Pressure-stabilized polymerization of nitrogen in alkaline-earth-metal strontium nitrides. Physical Chemistry Chemical Physics, 2020, 22, 5242-5248.	1.3	25
30	Proposed Superconducting Electride <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Li</mml:mi></mml:mrow><mml:mrow><mml:mn>6</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math> by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:mi>p</mml:mi></mml:mrow></mml:math> -Hybridized Cage States at Moderate Pressures. Physical Review Letters, 2021, 127, 157002.	2.9	25
31	Predicted structures and superconductivity of hypothetical Mg-CH4compounds under high pressures. Materials Research Express, 2015, 2, 046001.	0.8	24
32	Formation of twelve-fold iodine coordination at high pressure. Nature Communications, 2022, 13, 412.	5.8	23
33	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. Inorganic Chemistry, 2018, 57, 181-186.	1.9	22
34	Environment-dependent edge reconstruction of transition metal dichalcogenides: a global search. Materials Today Advances, 2020, 8, 100079.	2.5	21
35	Predicted Formation of H₃⁺ in Solid Halogen Polyhydrides at High Pressures. Journal of Physical Chemistry A, 2015, 119, 11059-11065.	1.1	19
36	Ground state structures of tantalum tetraboride and triboride: an ab initio study. Physical Chemistry Chemical Physics, 2016, 18, 18074-18080.	1.3	19

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37	Metallic and anti-metallic properties of strongly covalently bonded energetic AlN5 nitrides. Physical Chemistry Chemical Physics, 2019, 21, 12029-12035.	1.3	19
38	High-pressure close-packed structure of boron. RSC Advances, 2014, 4, 203-207.	1.7	18
39	Polymerization of Nitrogen in Ammonium Azide at High Pressures. Journal of Physical Chemistry C, 2015, 119, 25268-25272.	1.5	17
40	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.	0.9	17
41	Investigation of stable germane structures under high-pressure. Physical Chemistry Chemical Physics, 2015, 17, 27630-27635.	1.3	16
42	High-Pressure Bonding Mechanism of Selenium Nitrides. Inorganic Chemistry, 2019, 58, 2397-2402.	1.9	16
43	Local Carbon Concentration Determines the Graphene Edge Structure. Journal of Physical Chemistry Letters, 2020, 11, 3451-3457.	2.1	16
44	Prediction of stoichiometric PoHn compounds: crystal structures and properties. RSC Advances, 2015, 5, 103445-103450.	1.7	15
45	Enhancement of Tc in the atomic phase of iodine-doped hydrogen at high pressures. Physical Chemistry Chemical Physics, 2015, 17, 32335-32340.	1.3	15
46	Synthesis and characterization of a strong ferromagnetic and high hardness intermetallic compound Fe₂B. Physical Chemistry Chemical Physics, 2020, 22, 27425-27432.	1.3	15
47	Two-dimensional C₅₆₇₈: a promising carbon-based high-performance lithium-ion battery anode. Materials Advances, 2021, 2, 398-402.	2.6	15
48	Edge reconstructions of black phosphorene: a global search. Nanoscale, 2021, 13, 4085-4091.	2.8	15
49	Structural, mechanical and electronic properties of Rh2B and RhB2: first-principles calculations. Scientific Reports, 2015, 5, 10500.	1.6	14
50	Strong covalent boron bonding induced extreme hardness of VB3. Journal of Alloys and Compounds, 2016, 688, 1101-1107.	2.8	14
51	Structural phase transition and bonding properties of high-pressure polymeric CaN3. RSC Advances, 2018, 8, 4314-4320.	1.7	14
52	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N6 anions. Communications Chemistry, 2020, 3, .	2.0	14
53	Ab initio investigation of CaO-ZnO alloys under high pressure. Scientific Reports, 2015, 5, 11003.	1.6	13
54	Ab initio structure determination of n-diamond. Scientific Reports, 2015, 5, 13447.	1.6	13

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55	Ab initio study of germanium-hydride compounds under high pressure. RSC Advances, 2015, 5, 19432-19438.	1.7	13
56	Carbon and Oxygen Coordinating Atoms Adjust Transition Metal Single-Atom Catalysts Based On Boron Nitride Monolayers for Highly Efficient CO₂ Electroreduction. ACS Applied Materials & Interfaces, 2021, 13, 18934-18943.	4.0	13
57	Stability of hydrogen-terminated graphene edges. Physical Chemistry Chemical Physics, 2021, 23, 13261-13266.	1.3	11
58	Unraveling electrochemical CO reduction of the single-atom transition metals supported on N-doped phosphorene. Applied Surface Science, 2021, 545, 148953.	3.1	11
59	The crystal structure of IrB₂: a first-principle calculation. RSC Advances, 2014, 4, 63442-63446.	1.7	10
60	Pressure-induced phase transition of SnH₄: a new layered structure. RSC Advances, 2016, 6, 10456-10461.	1.7	10
61	Role of TMâ€“TM Connection Induced by Opposite d-Electron States on the Hardness of Transition-Metal (TM = Cr, W) Mononitrides. Inorganic Chemistry, 2019, 58, 15573-15579.	1.9	10
62	Anisotropic Angstrom-Wide Conductive Channels in Black Phosphorus by Top-down Cu Intercalation. Nano Letters, 2021, 21, 6336-6342.	4.5	10
63	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.	1.5	10
64	A novel stable hydrogen-rich SnH8 under high pressure. RSC Advances, 2015, 5, 107637-107641.	1.7	9
65	Ab initio study of native point defects in ZnO under pressure. Solid State Communications, 2015, 201, 130-134.	0.9	9
66	Revealing unusual rigid diamond net analogues in superhard titanium carbides. RSC Advances, 2018, 8, 14479-14487.	1.7	9
67	Ab initio studies of copper hydrides under high pressure. Frontiers of Physics, 2019, 14, 1.	2.4	9
68	Crystal structures and properties of the CH4H2compound under high pressure. RSC Advances, 2014, 4, 37569.	1.7	7
69	Structural and Electrical Properties of Be_xZn_{1â€“x}O Alloys under High Pressure. Chinese Physics Letters, 2021, 38, 026101.	1.3	7
70	High-pressure phase transition of MH3 (M: Er, Ho). Journal of Chemical Physics, 2014, 141, 054703.	1.2	6
71	First-principles study of ternary Li-Al-Te compounds under high pressure. Solid State Communications, 2018, 270, 58-64.	0.9	6
72	Structural and electrical properties of Gaâ€“Te systems under high pressure. Chinese Physics B, 2019, 28, 056104.	0.7	6

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73	First principle studies of ZnO1-xSx alloys under high pressure. Journal of Alloys and Compounds, 2019, 788, 905-911.	2.8	6
74	Structure and superconductivity of protactinium hydrides under high pressure. Journal of Physics Condensed Matter, 2019, 31, 315403.	0.7	6
75	Pressure-Induced Amorphization and Recrystallization of SnI₂. Journal of Physical Chemistry C, 2015, 119, 19312-19317.	1.5	5
76	Pressure-induced structural transformation of CaC2. Journal of Chemical Physics, 2016, 144, 194506.	1.2	5
77	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. Scientific Reports, 2016, 6, 18918.	1.6	5
78	Emergent property of high hardness for C-rich ruthenium carbides: partial covalent Ruâ€“Ru bonds. Physical Chemistry Chemical Physics, 2018, 20, 6108-6115.	1.3	5
79	High pressure superconducting phase of BI3: an ab initio study. RSC Advances, 2014, 4, 32068-32074.	1.7	4
80	Insights into Antibonding Induced Energy Density Enhancement and Exotic Electronic Properties for Germanium Nitrides at Modest Pressures. Inorganic Chemistry, 2018, 57, 10416-10423.	1.9	4
81	Defects of monolayer PbI₂: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 20553-20559.	1.3	4
82	Ab initio studies on ammonium iodine under high pressure. Chinese Physics B, 2020, 29, 053104.	0.7	4
83	H_d-Graphene: A Hexagon-Deficient Carbon-Based Anode for Metal-Ion Batteries with High Charge/Discharge Rates. ACS Applied Electronic Materials, 2021, 3, 5147-5154.	2.0	4
84	Crystal structures and properties of nitrogen oxides under high pressure. RSC Advances, 2015, 5, 103373-103379.	1.7	3
85	Ab initio study on the stability of N-doped ZnO under high pressure. RSC Advances, 2015, 5, 16774-16779.	1.7	3
86	Ground State Structures of Boron-Rich Rhodium Boride: An Ab Initio Study. Chinese Physics Letters, 2018, 35, 016401.	1.3	3
87	High-pressure structures of helium and carbon dioxide from first-principles calculations. Solid State Communications, 2018, 283, 9-13.	0.9	3
88	Structural, Electronic, and Optical Properties of ZnO_{1â€‰â€“â€‰x}Te_x Alloys. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1900155.	1.2	3
89	High-pressure formation of antimony nitrides: a first-principles study. RSC Advances, 2020, 10, 2448-2452.	1.7	3
90	Two-dimensional few-layered Janus diamond nanofilms with boron-terminated surfaces: First-principles calculation. Thin Solid Films, 2021, 722, 138570.	0.8	3

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91	Structural diversity and hydrogen storage properties in the system Kâ€“Siâ€“H. Physical Chemistry Chemical Physics, 2022, 24, 13033-13039.	1.3	3
92	Revealing the Role of d-Orbital Occupation in Edge Reconstruction of 1T-Transition-Metal Dichalcogenides. Journal of Physical Chemistry C, 2022, 126, 11389-11399.	1.5	3
93	A theoretical investigation on phase transition and dissociation of ammonium bromide under high pressure. Science Bulletin, 2014, 59, 5272-5277.	1.7	2
94	The hardness mechanism and bonding properties of CrN2: A first principle study. Computational Materials Science, 2019, 158, 282-288.	1.4	2
95	Stable structures and superconductivity of an Atâ€“H system at high pressure. Physical Chemistry Chemical Physics, 2018, 20, 24783-24789.	1.3	1
96	Strain-engineering enables reversible semiconductorâ€“metal transition of skutterudite IrAs3. Inorganic Chemistry Frontiers, 2020, 7, 1108-1114.	3.0	1
97	First-principle studies on the Liâ€“Te system. Materials Research Express, 2017, 4, 015701.	0.8	0
98	High pressure structural stability of the Na-Te system. AIP Advances, 2018, 8, 035123.	0.6	0
99	Strain engineering induced indirect-direct band gap transition of difluorphosphorane. Solid State Communications, 2020, 311, 113873.	0.9	0