

Da Li

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.

96
papers

1,818
citations

19
h-index

40
g-index

106
ext. papers

2,340
ext. citations

4.2
avg, IF

4.64
L-index

#	Paper	IF	Citations
96	Formation of twelve-fold iodine coordination at high pressure.. <i>Nature Communications</i> , 2022 , 13, 412	17.4	4
95	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
94	Two-dimensional few-layered Janus diamond nanofilms with boron-terminated surfaces: First-principles calculation. <i>Thin Solid Films</i> , 2021 , 722, 138570	2.2	2
93	Unraveling electrochemical CO reduction of the single-atom transition metals supported on N-doped phosphorene. <i>Applied Surface Science</i> , 2021 , 545, 148953	6.7	2
92	Carbon and Oxygen Coordinating Atoms Adjust Transition Metal Single-Atom Catalysts Based On Boron Nitride Monolayers for Highly Efficient CO Electroreduction. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 18934-18943	9.5	2
91	Anisotropic Angstrom-Wide Conductive Channels in Black Phosphorus by Top-down Cu Intercalation. <i>Nano Letters</i> , 2021 , 21, 6336-6342	11.5	5
90	Two-dimensional C5678: a promising carbon-based high-performance lithium-ion battery anode. <i>Materials Advances</i> , 2021 , 2, 398-402	3.3	3
89	Edge reconstructions of black phosphorene: a global search. <i>Nanoscale</i> , 2021 , 13, 4085-4091	7.7	4
88	Defects of monolayer Pbl: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 20553-20559	9.5	2
87	Stability of hydrogen-terminated graphene edges. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 13261-13266	3.2	3
86	Structural and Electrical Properties of Be x Zn1-x O Alloys under High Pressure. <i>Chinese Physics Letters</i> , 2021 , 38, 026101	1.8	2
85	Correlations of Ionic Migration and Deep-Level Traps Leads to Surface Defect Formation in Perovskite Solar Cells. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 19551-19559	3.8	1
84	Moderate Pressure Stabilized Pentazolate Cyclo-N Anion in Zn(N) Salt. <i>Inorganic Chemistry</i> , 2020 , 59, 8002-8012	5.1	15
83	Strain engineering induced indirect-direct band gap transition of difluorophosphorane. <i>Solid State Communications</i> , 2020 , 311, 113873	1.6	
82	High-pressure formation of antimony nitrides: a first-principles study.. <i>RSC Advances</i> , 2020 , 10, 2448-2453	3.7	1
81	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N6 anions. <i>Communications Chemistry</i> , 2020 , 3,	6.3	4
80	Ab initio studies on ammonium iodine under high pressure. <i>Chinese Physics B</i> , 2020 , 29, 053104	1.2	2

79	Pressure-stabilized polymerization of nitrogen in alkaline-earth-metal strontium nitrides. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 5242-5248	3.6	6
78	Strain-engineering enables reversible semiconductor-metal transition of skutterudite IrAs ₃ . <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 1108-1114	6.8	1
77	Synthesis and characterization of a strong ferromagnetic and high hardness intermetallic compound FeB. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 27425-27432	3.6	3
76	Environment-dependent edge reconstruction of transition metal dichalcogenides: a global search. <i>Materials Today Advances</i> , 2020 , 8, 100079	7.4	9
75	Local Carbon Concentration Determines the Graphene Edge Structure. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3451-3457	6.4	10
74	High-Pressure Bonding Mechanism of Selenium Nitrides. <i>Inorganic Chemistry</i> , 2019 , 58, 2397-2402	5.1	9
73	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
72	Structural and electrical properties of Ga _{1-x} In _x systems under high pressure. <i>Chinese Physics B</i> , 2019 , 28, 056104	1.2	3
71	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
70	Ab initio studies of copper hydrides under high pressure. <i>Frontiers of Physics</i> , 2019 , 14, 1	3.7	6
69	High-temperature superconductivity in ternary clathrate YCaH under high pressures. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 245404	1.8	10
68	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. <i>Inorganic Chemistry</i> , 2019 , 58, 2558-2564	5.1	12
67	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
66	Ternary superconducting phosphorus hydrides stabilized via lithium. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	13
65	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
64	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
63	Structure and superconductivity of protactinium hydrides under high pressure. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 315403	1.8	4
62	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

61	Ground State Structures of Boron-Rich Rhodium Boride: An Ab Initio Study. <i>Chinese Physics Letters</i> , 2018 , 35, 016401	1.8	2
60	Revealing unusual rigid diamond net analogues in superhard titanium carbides.. <i>RSC Advances</i> , 2018 , 8, 14479-14487	3.7	4
59	High pressure structural stability of the Na-Te system. <i>AIP Advances</i> , 2018 , 8, 035123	1.5	
58	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
57	Structural phase transition and bonding properties of high-pressure polymeric CaN ₃ . <i>RSC Advances</i> , 2018 , 8, 4314-4320	3.7	6
56	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. <i>Inorganic Chemistry</i> , 2018 , 57, 181-186	5.1	19
55	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
54	Pressure-induced superconducting ternary hydride H ₃ SXe: A theoretical investigation. <i>Frontiers of Physics</i> , 2018 , 13, 1	3.7	16
53	First-principles study of ternary Li-Al-Te compounds under high pressure. <i>Solid State Communications</i> , 2018 , 270, 58-64	1.6	3
52	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
51	High-pressure structures of helium and carbon dioxide from first-principles calculations. <i>Solid State Communications</i> , 2018 , 283, 9-13	1.6	2
50	First-principle studies on the LiTe system. <i>Materials Research Express</i> , 2017 , 4, 015701	1.7	
49	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
48	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
47	Bonding Properties of Aluminum Nitride at High Pressure. <i>Inorganic Chemistry</i> , 2017 , 56, 7494-7500	5.1	22
46	Stability of Sulfur Nitrides: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1515-1520	3.8	22
45	Divergent synthesis routes and superconductivity of ternary hydride MgSiH ₆ at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	32
44	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

43	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. <i>Scientific Reports</i> , 2016 , 6, 18918	4.9	5
42	Strong covalent boron bonding induced extreme hardness of VB3. <i>Journal of Alloys and Compounds</i> , 2016 , 688, 1101-1107	5.7	9
41	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
40	Pressure-induced phase transition of SnH4: a new layered structure. <i>RSC Advances</i> , 2016 , 6, 10456-10461	3.7	6
39	Stability and properties of the Ru-H system at high pressure. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1516-20	3.6	20
38	Pressure-induced structural transformation of CaC2. <i>Journal of Chemical Physics</i> , 2016 , 144, 194506	3.9	4
37	High pressure structures and superconductivity of AlH3(H2) predicted by first principles. <i>RSC Advances</i> , 2015 , 5, 5096-5101	3.7	26
36	Pressure-Induced Amorphization and Recrystallization of SnI2. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 19312-19317	3.8	4
35	Structural, mechanical, and electronic properties of Rh2B and RhB2: first-principles calculations. <i>Scientific Reports</i> , 2015 , 5, 10500	4.9	10
34	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
33	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. <i>Scientific Reports</i> , 2015 , 5, 11381	4.9	18
32	Ab initio study of germanium-hydride compounds under high pressure. <i>RSC Advances</i> , 2015 , 5, 19432-19438	3.8	12
31	Cubic C96: a novel carbon allotrope with a porous nanocube network. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 10448-10452	13	38
30	Polymerization of Nitrogen in Ammonium Azide at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 25268-25272	3.8	14
29	Pressure-Induced Structures and Properties in Indium Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 9924-8	5.1	23
28	Investigation of stable germane structures under high-pressure. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 27630-5	3.6	13
27	Ab initio study of native point defects in ZnO under pressure. <i>Solid State Communications</i> , 2015 , 201, 130-134	1.6	7
26	Prediction of stoichiometric PoHn compounds: crystal structures and properties. <i>RSC Advances</i> , 2015 , 5, 103445-103450	3.7	12

25	Pressure-induced decomposition of solid hydrogen sulfide. <i>Physical Review B</i> , 2015 , 91,	3.3	213
24	Ab initio investigation of CaO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2015 , 5, 11003	4.9	11
23	Ab initio structure determination of n-diamond. <i>Scientific Reports</i> , 2015 , 5, 13447	4.9	12
22	High-temperature superconductivity in compressed solid silane. <i>Scientific Reports</i> , 2015 , 5, 8845	4.9	18
21	Predicted structures and superconductivity of hypothetical Mg-CH ₄ compounds under high pressures. <i>Materials Research Express</i> , 2015 , 2, 046001	1.7	16
20	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
19	Crystal structures and properties of nitrogen oxides under high pressure. <i>RSC Advances</i> , 2015 , 5, 103373-103379	3.7	10
18	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
17	A novel stable hydrogen-rich SnH ₈ under high pressure. <i>RSC Advances</i> , 2015 , 5, 107637-107641	3.7	6
16	Ab initio study on the stability of N-doped ZnO under high pressure. <i>RSC Advances</i> , 2015 , 5, 16774-16779	3.7	2
15	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2014 , 4, 5759	4.9	19
14	Pressure-induced metallization of dense (H ₂) ₂ with high-T _c superconductivity. <i>Scientific Reports</i> , 2014 , 4, 6968	4.9	502
13	Nitrogen concentration driving the hardness of rhenium nitrides. <i>Scientific Reports</i> , 2014 , 4, 4797	4.9	47
12	High-pressure close-packed structure of boron. <i>RSC Advances</i> , 2014 , 4, 203-207	3.7	17
11	A theoretical investigation on phase transition and dissociation of ammonium bromide under high pressure. <i>Science Bulletin</i> , 2014 , 59, 5272-5277		2
10	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. <i>RSC Advances</i> , 2014 , 4, 10133	3.7	52
9	High pressure superconducting phase of Bi ₃ : an ab initio study. <i>RSC Advances</i> , 2014 , 4, 32068-32074	3.7	3
8	Modulated T carbon-like carbon allotropes: an ab initio study. <i>RSC Advances</i> , 2014 , 4, 17364	3.7	28

7	Crystal structures and properties of the CH ₄ H ₂ compound under high pressure. <i>RSC Advances</i> , 2014 , 4, 37569	3.7	6
6	Ultrahard boron-rich tantalum boride: Monoclinic TaB ₄ . <i>Journal of Alloys and Compounds</i> , 2014 , 617, 660-664	5.7	16
5	High-pressure phase transition of MH ₂ (M: Er, Ho). <i>Journal of Chemical Physics</i> , 2014 , 141, 054703	3.9	4
4	The crystal structure of IrB ₂ : a first-principle calculation. <i>RSC Advances</i> , 2014 , 4, 63442-63446	3.7	10
3	Large Volume Collapse during Pressure-Induced Phase Transition in Lithium Amide. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 9744-9749	3.8	29
2	Lowest enthalpy polymorph of cold-compressed graphite phase. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4347-50	3.6	77
1	Cubic gauche-CN: A superhard metallic compound predicted via first-principles calculations. <i>Journal of Chemical Physics</i> , 2010 , 133, 044512	3.9	34