Fubo Tian

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/2084900/publications.pdf

Version: 2024-02-01

116 papers	3,063 citations	185998 28 h-index	174990 52 g-index
122 all docs	122 docs citations	122 times ranked	1960 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	Superhard semiconductingC3N2compounds predicted via first-principles calculations. Physical Review B, 2008, 78, .	1.1	60
8	Structural stability of polymeric nitrogen: A first-principles investigation. Journal of Chemical Physics, 2010, 132, 024502.	1.2	60
9	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
10	New Metallic Ordered Phase of Perovskite CsPbI₃ under Pressure. Advanced Science, 2019, 6, 1900399.	5.6	57
11	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. RSC Advances, 2014, 4, 10133.	1.7	55
12	Cubic C₉₆: a novel carbon allotrope with a porous nanocube network. Journal of Materials Chemistry A, 2015, 3, 10448-10452.	5.2	47
13	Hydrogen bond symmetrization and superconducting phase of HBr and HCl under high pressure: An ab initio study. Journal of Chemical Physics, 2010, 133, 074509.	1.2	41
14	Cubic gauche-CN: A superhard metallic compound predicted via first-principles calculations. Journal of Chemical Physics, 2010, 133, 044512.	1.2	40
15	Prediction of superconducting ternary hydride MgGeH₆: from divergent high-pressure formation routes. Physical Chemistry Chemical Physics, 2017, 19, 27406-27412.	1.3	40
16	Ternary superconducting cophosphorus hydrides stabilized via lithium. Npj Computational Materials, 2019, 5, .	3.5	38
17	Scandiumâ€Doped AlN 1D Hexagonal Nanoprisms: A Class of Roomâ€Temperature Ferromagnetic Materials. Angewandte Chemie - International Edition, 2010, 49, 173-176.	7.2	36
18	Pressure-Induced Structures and Properties in Indium Hydrides. Inorganic Chemistry, 2015, 54, 9924-9928.	1.9	34

#	Article	IF	Citations
19	Bonding Properties of Aluminum Nitride at High Pressure. Inorganic Chemistry, 2017, 56, 7494-7500.	1.9	34
20	High pressure structures and superconductivity of AlH₃(H₂) predicted by first principles. RSC Advances, 2015, 5, 5096-5101.	1.7	33
21	Potentially superhard hcp<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cr</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>compound studied at high pressure. Physical Review B, 2016, 93, .	1.1	33
22	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. Inorganic Chemistry, 2019, 58, 2558-2564.	1.9	33
23	Two-dimensional ferromagnetic semiconductors of rare-earth monolayer GdX2 (XÂ= Cl, Br, I) with large perpendicular magnetic anisotropy and high Curie temperature. Materials Today Physics, 2021, 21, 100514.	2.9	32
24	High-temperature superconductivity in ternary clathrate YCaH₁₂ under high pressures. Journal of Physics Condensed Matter, 2019, 31, 245404.	0.7	31
25	Moderate Pressure Stabilized Pentazolate Cyclo-N₅^{â€“} Anion in Zn(N₅)₂ Salt. Inorganic Chemistry, 2020, 59, 8002-8012.	1.9	31
26	A new phase of solid iodine with different molecular covalent bonds. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 4999-5001.	3.3	30
27	Stability of Sulfur Nitrides: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 1515-1520.	1.5	30
28	Modulated T carbon-like carbon allotropes: an ab initio study. RSC Advances, 2014, 4, 17364.	1.7	29
29	Structures and Properties of Osmium Hydrides under Pressure from First Principle Calculation. Journal of Physical Chemistry C, 2015, 119, 15905-15911.	1.5	29
30	Ultrahard boron-rich tantalum boride: Monoclinic TaB 4. Journal of Alloys and Compounds, 2014, 617, 660-664.	2.8	28
31	Phase diagram, mechanical properties, and electronic structure of Nbâ€“N compounds under pressure. Physical Chemistry Chemical Physics, 2015, 17, 22837-22845.	1.3	27
32	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. Scientific Reports, 2014, 4, 5759.	1.6	26
33	First-principles study on the structural and electronic properties of metallic HfH2 under pressure. Scientific Reports, 2015, 5, 11381.	1.6	26
34	Stability and properties of the Ruâ€“H system at high pressure. Physical Chemistry Chemical Physics, 2016, 18, 1516-1520.	1.3	26
35	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></m 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
36	Predicted structures and superconductivity of hypothetical Mg-CH4compounds under high pressures. Materials Research Express, 2015, 2, 046001.	0.8	24

#	Article	IF	Citations
37	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. Physical Chemistry Chemical Physics, 2015, 17, 13397-13402.	1.3	23
38	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. Inorganic Chemistry, 2018, 57, 181-186.	1.9	22
39	Predicted novel metallic metastable phases of polymeric nitrogen at high pressures. New Journal of Physics, 2013, 15, 013010.	1.2	19
40	Predicted Formation of H₃⁺ in Solid Halogen Polyhydrides at High Pressures. Journal of Physical Chemistry A, 2015, 119, 11059-11065.	1.1	19
41	Ground state structures of tantalum tetraboride and triboride: an ab initio study. Physical Chemistry Chemical Physics, 2016, 18, 18074-18080.	1.3	19
42	Metallic and anti-metallic properties of strongly covalently bonded energetic AlN5 nitrides. Physical Chemistry Chemical Physics, 2019, 21, 12029-12035.	1.3	19
43	Pressure induced phase transition in MH2 (M = V, Nb). Journal of Chemical Physics, 2014, 140, 114703.	1.2	18
44	High-pressure close-packed structure of boron. RSC Advances, 2014, 4, 203-207.	1.7	18
45	Order-disorder phase transition and dissociation of hydrogen sulfide under high pressure: Ab initio molecular dynamics study. Journal of Chemical Physics, 2010, 132, 164506.	1.2	17
46	Polymerization of Nitrogen in Ammonium Azide at High Pressures. Journal of Physical Chemistry C, 2015, 119, 25268-25272.	1.5	17
47	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
48	Hydrogen-bond enhancement triggered structural evolution and band gap engineering of hybrid perovskite (C₆H₅CH₂NH₃)₂PbI₄ under high pressure. Physical Chemistry Chemical Physics, 2020, 22, 1841-1846.	1.3	17
49	High-Pressure Bonding Mechanism of Selenium Nitrides. Inorganic Chemistry, 2019, 58, 2397-2402.	1.9	16
50	Prediction of stoichiometric PoHn compounds: crystal structures and properties. RSC Advances, 2015, 5, 103445-103450.	1.7	15
51	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
52	Structural, mechanical and electronic properties of Rh2B and RhB2: first-principles calculations. Scientific Reports, 2015, 5, 10500.	1.6	14
53	Strong covalent boron bonding induced extreme hardness of VB3. Journal of Alloys and Compounds, 2016, 688, 1101-1107.	2.8	14
54	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N6 anions. Communications Chemistry, 2020, 3, .	2.0	14

#	Article	IF	Citations
55	Ab initio investigation of CaO-ZnO alloys under high pressure. Scientific Reports, 2015, 5, 11003.	1.6	13
56	Ab initio structure determination of n-diamond. Scientific Reports, 2015, 5, 13447.	1.6	13
57	Effects of magnetic ordering and electron correlations on the stability of FeN. RSC Advances, 2015, 5, 31270-31274.	1.7	13
58	Ab initio study of germanium-hydride compounds under high pressure. RSC Advances, 2015, 5, 19432-19438.	1.7	13
59	Pressure-induced phase transitions and insulator-metal transitions in VO2 nanoparticles. Journal of Alloys and Compounds, 2017, 709, 260-266.	2.8	12
60	Unexpected magnetic coupling oscillations for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>L</mml:mi><mml:msub><mml:mn>1</mml:mn> films induced by quantum wells. Physical Review B, 2018, 97, .	1.4	12
61	Enhanced resistive switching performance in yttrium-doped CH₃NH₃PbI₃ perovskite devices. Physical Chemistry Chemical Physics, 2021, 23, 21757-21768.	1.3	12
62	The crystal structure and superconducting properties of monatomic bromine. Journal of Physics Condensed Matter, 2010, 22, 015702.	0.7	10
63	The crystal structure of IrB₂: a first-principle calculation. RSC Advances, 2014, 4, 63442-63446.	1.7	10
64	High and reversible spin polarization in a collinear antiferromagnet. Applied Physics Reviews, 2020, 7, .	5.5	10
65	A New Superconducting 3R-WS₂ Phase at High Pressure. Journal of Physical Chemistry Letters, 2021, 12, 3321-3327.	2.1	10
66	The stability, electronic properties, and hardness of SiN2 under high pressure. RSC Advances, 2014, 4, 55023-55027.	1.7	9
67	Ab initio study of native point defects in ZnO under pressure. Solid State Communications, 2015, 201, 130-134.	0.9	9
68	Revealing unusual rigid diamond net analogues in superhard titanium carbides. RSC Advances, 2018, 8, 14479-14487.	1.7	9
69	Ab initio study of vacancies in cubic BN under pressure. Solid State Communications, 2007, 143, 532-536.	0.9	8
70	Superconductive superhard phase of BC7: Predicted via ab initio calculations. Diamond and Related Materials, 2011, 20, 454-457.	1.8	7
71	Crystal structures and properties of the CH4H2compound under high pressure. RSC Advances, 2014, 4, 37569.	1.7	7
72	Structural and Electrical Properties of Be_xZn_{1â€“x}O Alloys under High Pressure. Chinese Physics Letters, 2021, 38, 026101.	1.3	7

#	Article	IF	Citations
73	Full-Electrical Writing and Reading of Magnetization States in a Magnetic Junction with Symmetrical Structure and Antiparallel Magnetic Configuration. ACS Nano, 2021, 15, 12213-12221.	7.3	7
74	Interfacial antiferromagnetic coupling and high spin polarization in metallic phthalocyanines. Physical Review B, 2021, 103, .	1.1	7
75	Structural, electronic, and optical properties of crystalline iodoform under high pressure: A first-principles study. Journal of Chemical Physics, 2011, 134, 034508.	1.2	6
76	High-pressure phase transition of MH3 (M: Er, Ho). Journal of Chemical Physics, 2014, 141, 054703.	1.2	6
77	First-principles study of ternary Li-Al-Te compounds under high pressure. Solid State Communications, 2018, 270, 58-64.	0.9	6
78	Structural and electrical properties of Gaâ€“Te systems under high pressure. Chinese Physics B, 2019, 28, 056104.	0.7	6
79	First principle studies of ZnO1-xSx alloys under high pressure. Journal of Alloys and Compounds, 2019, 788, 905-911.	2.8	6
80	Structure and superconductivity of protactinium hydrides under high pressure. Journal of Physics Condensed Matter, 2019, 31, 315403.	0.7	6
81	Near-edge X-ray absorption fine structure of solid oxygen under high pressure: A density functional theory study. Solid State Communications, 2008, 147, 126-129.	0.9	5
82	New high-pressure phase of BaH2predicted byab initiostudies. Journal of Physics Condensed Matter, 2010, 22, 225401.	0.7	5
83	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. Scientific Reports, 2016, 6, 18918.	1.6	5
84	Magnetic Improvement and Relaxation Mechanism of the Tb-Phthalocyanine Single-Molecule Magnet by Absorbing CH₂Cl₂ Molecules. Journal of Physical Chemistry C, 2021, 125, 10165-10172.	1.5	5
85	High pressure superconducting phase of BI3: an ab initio study. RSC Advances, 2014, 4, 32068-32074.	1.7	4
86	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
87	Unusual interfacial magnetic interactions for Ï„-MnAl with Fe(Co) atomic layers. Physical Chemistry Chemical Physics, 2019, 21, 2443-2452.	1.3	4
88	Ab initio studies on ammonium iodine under high pressure. Chinese Physics B, 2020, 29, 053104.	0.7	4
89	First-principles supercell studies of the substitutional carbon in c-BN. Diamond and Related Materials, 2008, 17, 2025-2028.	1.8	3
90	Highâ€pressure phase transitions in NaBH₄ from firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 1139-1142.	0.7	3

#	Article	IF	Citations
91	Crystal structures and properties of nitrogen oxides under high pressure. RSC Advances, 2015, 5, 103373-103379.	1.7	3
92	Ab initio study on the stability of N-doped ZnO under high pressure. RSC Advances, 2015, 5, 16774-16779.	1.7	3
93	High-pressure structures of helium and carbon dioxide from first-principles calculations. Solid State Communications, 2018, 283, 9-13.	0.9	3
94	Metallization: New Metallic Ordered Phase of Perovskite CsPbI3 under Pressure (Adv. Sci. 14/2019). Advanced Science, 2019, 6, 1970083.	5.6	3
95	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
96	First principles study on the structures and properties of SnOâ€“ZnO alloys under high pressure. Materials Science in Semiconductor Processing, 2022, 144, 106566.	1.9	3
97	Structural diversity and hydrogen storage properties in the system Kâ€“Siâ€“H. Physical Chemistry Chemical Physics, 2022, 24, 13033-13039.	1.3	3
98	High-pressure phase transitions of Cu 2 O. Solid State Sciences, 2017, 74, 70-73.	1.5	2
99	Charge-patching method for the calculation of electronic structure of polypeptides. Physical Chemistry Chemical Physics, 2018, 20, 23301-23310.	1.3	2
100	The hardness mechanism and bonding properties of CrN2: A first principle study. Computational Materials Science, 2019, 158, 282-288.	1.4	2
101	Synthesis of superconducting SbS and SbS2 antimony chalcogenide compounds at high pressures. Physical Review B, 2021, 103, .	1.1	2
102	Effect of Ta capping layer on the magnetic coupling oscillation of L10-MnGa/Co/Ta films. Journal of Magnetism and Magnetic Materials, 2020, 511, 166994.	1.0	2
103	Dirac nodal-line semimetal zinc polynitride at high pressure. Physical Review B, 2022, 105, .	1.1	2
104	Pressure-induced formation of hydrogen bonds in KNH₂ studied by first principles. RSC Advances, 2016, 6, 78678-78683.	1.7	1
105	Stable structures and superconductivity of an Atâ€“H system at high pressure. Physical Chemistry Chemical Physics, 2018, 20, 24783-24789.	1.3	1
106	Variational and diffusion Monte Carlo simulations of a hydrogen molecular ion in a spherical box*. Chinese Physics B, 2019, 28, 056401.	0.7	1
107	Magnetic coupling in L10-MnGa/Ni films. Materials Research Express, 2019, 6, 116414.	0.8	1
108	Strain-engineering enables reversible semiconductorâ€“metal transition of skutterudite IrAs3. Inorganic Chemistry Frontiers, 2020, 7, 1108-1114.	3.0	1

#	Article	IF	Citations
109	Interfacial magnetic coupling and orbital hybridization for D022-Mn3Ga/Fe films. Physica Scripta, 2021, 96, 075804.	1.2	1
110	First-principle studies on the Liâ€“Te system. Materials Research Express, 2017, 4, 015701.	0.8	0
111	High pressure structural stability of the Na-Te system. AIP Advances, 2018, 8, 035123.	0.6	0
112	Interfacial magnetic coupling and the confinement effect of spin electrons for Ï„-MnAl/Ni multilayers. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126096.	0.9	0
113	Pressure-induced the formation of Mg(CH3)2 and Ca(CH3)2 studied by the first principles. Solid State Communications, 2020, 320, 114027.	0.9	0
114	First principle studies of ammonium chloride under high pressure. RSC Advances, 2021, 11, 5149-5155.	1.7	0
115	The new valence state [Ga]â^'5 in Li-Ga-Te system under high pressure. Solid State Communications, 2021, 336, 114402.	0.9	0
116	Breaking the symmetry of spin-sublattices in antiferromagnet by interfacial tailoring in the L10-MnPt/NaCl/Fe junction. Applied Physics Letters, 2021, 119, 172401.	1.5	0