

Fubo Tian

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.

113 papers	2,097 citations	22 h-index	42 g-index
122 ext. papers	2,597 ext. citations	4.2 avg, IF	4.63 L-index

#	Paper	IF	Citations
113	First principles study on the structures and properties of SnO ₂ /ZnO alloys under high pressure. <i>Materials Science in Semiconductor Processing</i> , 2022 , 144, 106566	4.3	0
112	Breaking the symmetry of spin-sublattices in antiferromagnet by interfacial tailoring in the L10-MnPt/NaCl/Fe junction. <i>Applied Physics Letters</i> , 2021 , 119, 172401	3.4	
111	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
110	A New Superconducting 3R-WS Phase at High Pressure. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 3321-3327	6.4	2
109	Magnetic Improvement and Relaxation Mechanism of the Tb-Phthalocyanine Single-Molecule Magnet by Absorbing CH ₂ Cl ₂ Molecules. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 10165-10172	3.8	3
108	Interfacial magnetic coupling and orbital hybridization for D022-Mn ₃ Ga/Fe films. <i>Physica Scripta</i> , 2021 , 96, 075804	2.6	0
107	First principle studies of ammonium chloride under high pressure.. <i>RSC Advances</i> , 2021 , 11, 5149-5155	3.7	
106	Structural and Electrical Properties of Be _x Zn _{1-x} O Alloys under High Pressure. <i>Chinese Physics Letters</i> , 2021 , 38, 026101	1.8	2
105	Full-Electrical Writing and Reading of Magnetization States in a Magnetic Junction with Symmetrical Structure and Antiparallel Magnetic Configuration. <i>ACS Nano</i> , 2021 ,	16.7	1
104	The new valence state [Ga] ⁵⁺ in Li-Ga-Te system under high pressure. <i>Solid State Communications</i> , 2021 , 336, 114402	1.6	
103	Two-dimensional ferromagnetic semiconductors of rare-earth monolayer GdX ₂ (X = Cl, Br, I) with large perpendicular magnetic anisotropy and high Curie temperature. <i>Materials Today Physics</i> , 2021 , 21, 100514	8	8
102	Interfacial antiferromagnetic coupling and high spin polarization in metallic phthalocyanines. <i>Physical Review B</i> , 2021 , 103,	3.3	5
101	Enhanced resistive switching performance in yttrium-doped CHNHPbI perovskite devices. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 21757-21768	3.6	2
100	Moderate Pressure Stabilized Pentazolate Cyclo-N Anion in Zn(N) Salt. <i>Inorganic Chemistry</i> , 2020 , 59, 8002-8012	5.1	15
99	Hydrogen-bond enhancement triggered structural evolution and band gap engineering of hybrid perovskite (CH ₃ CH ₂ NH ₃)PbI ₃ under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 1841-1846	3.6	8
98	Formation mechanism of insensitive tellurium hexanitride with armchair-like cyclo-N ₆ anions. <i>Communications Chemistry</i> , 2020 , 3,	6.3	4
97	Effect of Ta capping layer on the magnetic coupling oscillation of L10-MnGa/Co/Ta films. <i>Journal of Magnetism and Magnetic Materials</i> , 2020 , 511, 166994	2.8	2

96	Ab initio studies on ammonium iodine under high pressure. <i>Chinese Physics B</i> , 2020 , 29, 053104	1.2	2
95	Interfacial magnetic coupling and the confinement effect of spin electrons for EMnAl/Ni multilayers. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020 , 384, 126096	2.3	
94	Strain-engineering enables reversible semiconductor-metal transition of skutterudite IrAs ₃ . <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 1108-1114	6.8	1
93	Pressure-induced the formation of Mg(CH ₃) ₂ and Ca(CH ₃) ₂ studied by the first principles. <i>Solid State Communications</i> , 2020 , 320, 114027	1.6	
92	High and reversible spin polarization in a collinear antiferromagnet. <i>Applied Physics Reviews</i> , 2020 , 7, 031405	17.3	3
91	Unusual interfacial magnetic interactions for EMnAl with Fe(Co) atomic layers. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 2443-2452	3.6	3
90	High-Pressure Bonding Mechanism of Selenium Nitrides. <i>Inorganic Chemistry</i> , 2019 , 58, 2397-2402	5.1	9
89	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
88	Structural and electrical properties of GaTe systems under high pressure. <i>Chinese Physics B</i> , 2019 , 28, 056104	1.2	3
87	New Metallic Ordered Phase of Perovskite CsPbI ₃ under Pressure. <i>Advanced Science</i> , 2019 , 6, 1900399	13.6	33
86	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
85	High-temperature superconductivity in ternary clathrate YCaH under high pressures. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 245404	1.8	10
84	Unique Phase Diagram and Superconductivity of Calcium Hydrides at High Pressures. <i>Inorganic Chemistry</i> , 2019 , 58, 2558-2564	5.1	12
83	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
82	Metallization: New Metallic Ordered Phase of Perovskite CsPbI ₃ under Pressure (Adv. Sci. 14/2019). <i>Advanced Science</i> , 2019 , 6, 1970083	13.6	2
81	Variational and diffusion Monte Carlo simulations of a hydrogen molecular ion in a spherical box. <i>Chinese Physics B</i> , 2019 , 28, 056401	1.2	1
80	Magnetic coupling in L10-MnGa/Ni films. <i>Materials Research Express</i> , 2019 , 6, 116414	1.7	1
79	Ternary superconducting phosphorus hydrides stabilized via lithium. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	13

78	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
77	Structure and superconductivity of protactinium hydrides under high pressure. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 315403	1.8	4
76	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
75	Revealing unusual rigid diamond net analogues in superhard titanium carbides.. <i>RSC Advances</i> , 2018 , 8, 14479-14487	3.7	4
74	High pressure structural stability of the Na-Te system. <i>AIP Advances</i> , 2018 , 8, 035123	1.5	
73	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. <i>Inorganic Chemistry</i> , 2018 , 57, 181-186	5.1	19
72	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
71	Charge-patching method for the calculation of electronic structure of polypeptides. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 23301-23310	3.6	1
70	First-principles study of ternary Li-Al-Te compounds under high pressure. <i>Solid State Communications</i> , 2018 , 270, 58-64	1.6	3
69	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
68	Unexpected magnetic coupling oscillations for L ₁₀ MnGa/Co(Fe) films induced by quantum wells. <i>Physical Review B</i> , 2018 , 97,	3.3	10
67	High-pressure structures of helium and carbon dioxide from first-principles calculations. <i>Solid State Communications</i> , 2018 , 283, 9-13	1.6	2
66	First-principle studies on the LiTe system. <i>Materials Research Express</i> , 2017 , 4, 015701	1.7	
65	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
64	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
63	Bonding Properties of Aluminum Nitride at High Pressure. <i>Inorganic Chemistry</i> , 2017 , 56, 7494-7500	5.1	22
62	Pressure-induced phase transitions and insulator-metal transitions in VO ₂ nanoparticles. <i>Journal of Alloys and Compounds</i> , 2017 , 709, 260-266	5.7	8
61	Stability of Sulfur Nitrides: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1515-1520	3.8	22

60	High-pressure phase transitions of Cu ₂ O. <i>Solid State Sciences</i> , 2017 , 74, 70-73	3.4	1
59	Divergent synthesis routes and superconductivity of ternary hydride MgSiH ₆ at high pressure. <i>Physical Review B</i> , 2017 , 96,	3.3	32
58	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
57	Pressure-induced formation of hydrogen bonds in KNH ₂ studied by first principles. <i>RSC Advances</i> , 2016 , 6, 78678-78683	3.7	1
56	Ab initio molecular dynamic study of solid-state transitions of ammonium nitrate. <i>Scientific Reports</i> , 2016 , 6, 18918	4.9	5
55	Strong covalent boron bonding induced extreme hardness of VB ₃ . <i>Journal of Alloys and Compounds</i> , 2016 , 688, 1101-1107	5.7	9
54	Potentially superhard hcp CrN ₂ compound studied at high pressure. <i>Physical Review B</i> , 2016 , 93,	3.3	21
53	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
52	Stability and properties of the Ru-H system at high pressure. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1516-20	3.6	20
51	High pressure structures and superconductivity of AlH ₃ (H ₂) predicted by first principles. <i>RSC Advances</i> , 2015 , 5, 5096-5101	3.7	26
50	Phase diagram, mechanical properties, and electronic structure of Nb-N compounds under pressure. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 22837-45	3.6	20
49	Structural, mechanical, and electronic properties of Rh ₂ B and RhB ₂ : first-principles calculations. <i>Scientific Reports</i> , 2015 , 5, 10500	4.9	10
48	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
47	First-principles study on the structural and electronic properties of metallic HfH ₂ under pressure. <i>Scientific Reports</i> , 2015 , 5, 11381	4.9	18
46	Ab initio study of germanium-hydride compounds under high pressure. <i>RSC Advances</i> , 2015 , 5, 19432-19438	3.7	12
45	The low coordination number of nitrogen in hard tungsten nitrides: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 13397-402	3.6	19
44	Cubic C96: a novel carbon allotrope with a porous nanocube network. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 10448-10452	13	38
43	Polymerization of Nitrogen in Ammonium Azide at High Pressures. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 25268-25272	3.8	14

42	Pressure-Induced Structures and Properties in Indium Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 9924-8	5.1	23
41	Ab initio study of native point defects in ZnO under pressure. <i>Solid State Communications</i> , 2015 , 201, 130-134	1.6	7
40	Prediction of stoichiometric PoHn compounds: crystal structures and properties. <i>RSC Advances</i> , 2015 , 5, 103445-103450	3.7	12
39	Pressure-induced decomposition of solid hydrogen sulfide. <i>Physical Review B</i> , 2015 , 91,	3.3	213
38	Ab initio investigation of CaO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2015 , 5, 11003	4.9	11
37	Ab initio structure determination of n-diamond. <i>Scientific Reports</i> , 2015 , 5, 13447	4.9	12
36	Effects of magnetic ordering and electron correlations on the stability of FeN. <i>RSC Advances</i> , 2015 , 5, 31270-31274	3.7	13
35	Predicted structures and superconductivity of hypothetical Mg-CH ₄ compounds under high pressures. <i>Materials Research Express</i> , 2015 , 2, 046001	1.7	16
34	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
33	Crystal structures and properties of nitrogen oxides under high pressure. <i>RSC Advances</i> , 2015 , 5, 103373-103379	3.7	10
32	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
31	Ab initio study on the stability of N-doped ZnO under high pressure. <i>RSC Advances</i> , 2015 , 5, 16774-16779	3.7	2
30	Miscibility and ordered structures of MgO-ZnO alloys under high pressure. <i>Scientific Reports</i> , 2014 , 4, 5759	4.9	19
29	Pressure-induced metallization of dense (H ₂)B ₂ with high-T _c superconductivity. <i>Scientific Reports</i> , 2014 , 4, 6968	4.9	502
28	Nitrogen concentration driving the hardness of rhenium nitrides. <i>Scientific Reports</i> , 2014 , 4, 4797	4.9	47
27	High-pressure close-packed structure of boron. <i>RSC Advances</i> , 2014 , 4, 203-207	3.7	17
26	The stability, electronic properties, and hardness of SiN ₂ under high pressure. <i>RSC Advances</i> , 2014 , 4, 55023-55027	3.7	7
25	Mechanical and metallic properties of tantalum nitrides from first-principles calculations. <i>RSC Advances</i> , 2014 , 4, 10133	3.7	52

24	High pressure superconducting phase of Bi ₃ : an ab initio study. <i>RSC Advances</i> , 2014 , 4, 32068-32074	3.7	3
23	Modulated T carbon-like carbon allotropes: an ab initio study. <i>RSC Advances</i> , 2014 , 4, 17364	3.7	28
22	Crystal structures and properties of the CH ₄ H ₂ compound under high pressure. <i>RSC Advances</i> , 2014 , 4, 37569	3.7	6
21	Ultrahard boron-rich tantalum boride: Monoclinic TaB ₄ . <i>Journal of Alloys and Compounds</i> , 2014 , 617, 660-664	5.7	16
20	High-pressure phase transition of MH ₂ (M = Er, Ho). <i>Journal of Chemical Physics</i> , 2014 , 141, 054703	3.9	4
19	Pressure induced phase transition in MH ₂ (M = V, Nb). <i>Journal of Chemical Physics</i> , 2014 , 140, 114703	3.9	16
18	The crystal structure of IrB ₂ : a first-principle calculation. <i>RSC Advances</i> , 2014 , 4, 63442-63446	3.7	10
17	Predicted novel metallic metastable phases of polymeric nitrogen at high pressures. <i>New Journal of Physics</i> , 2013 , 15, 013010	2.9	13
16	Lowest enthalpy polymorph of cold-compressed graphite phase. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4347-50	3.6	77
15	Superconductive superhard phase of BC ₇ : Predicted via ab initio calculations. <i>Diamond and Related Materials</i> , 2011 , 20, 454-457	3.5	6
14	High-pressure phase transitions in NaBH ₄ from first-principles calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 1139-1142	1.3	3
13	Structural, electronic, and optical properties of crystalline iodoform under high pressure: a first-principles study. <i>Journal of Chemical Physics</i> , 2011 , 134, 034508	3.9	5
12	Cubic gauche-CN: A superhard metallic compound predicted via first-principles calculations. <i>Journal of Chemical Physics</i> , 2010 , 133, 044512	3.9	34
11	Order-disorder phase transition and dissociation of hydrogen sulfide under high pressure: ab initio molecular dynamics study. <i>Journal of Chemical Physics</i> , 2010 , 132, 164506	3.9	16
10	Hydrogen bond symmetrization and superconducting phase of HBr and HCl under high pressure: An ab initio study. <i>Journal of Chemical Physics</i> , 2010 , 133, 074509	3.9	37
9	New high-pressure phase of BaH ₂ predicted by ab initio studies. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 225401	1.8	5
8	The crystal structure and superconducting properties of monatomic bromine. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 015702	1.8	9
7	Structural stability of polymeric nitrogen: A first-principles investigation. <i>Journal of Chemical Physics</i> , 2010 , 132, 024502	3.9	48

6	Scandium-doped AlN 1D hexagonal nanoprisms: a class of room-temperature ferromagnetic materials. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 173-6	16.4	34
5	First-principles supercell studies of the substitutional carbon in c-BN. <i>Diamond and Related Materials</i> , 2008 , 17, 2025-2028	3.5	3
4	A new phase of solid iodine with different molecular covalent bonds. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 4999-5001	11.5	25
3	Superhard semiconducting C ₃ N ₂ compounds predicted via first-principles calculations. <i>Physical Review B</i> , 2008 , 78,	3.3	50
2	Near-edge X-ray absorption fine structure of solid oxygen under high pressure: A density functional theory study. <i>Solid State Communications</i> , 2008 , 147, 126-129	1.6	5
1	Ab initio study of vacancies in cubic BN under pressure. <i>Solid State Communications</i> , 2007 , 143, 532-536	1.6	7