Bao-Tian Wang

List of Publications by Citations

99 papers	1,805 citations	26 h-index	37 g-index
114 ext. papers	2,436 ext. citations	4.7 avg, IF	5.19 L-index

#	Paper	IF	Citations
99	Ground-state properties and high-pressure behavior of plutonium dioxide: Density functional theory calculations. *Physical Review B*, **2010**, 82,	3.3	105
98	Structural and mechanistic revelations on high capacity cation-disordered Li-rich oxides for rechargeable Li-ion batteries. *Energy Storage Materials*, **2019**, 16, 354-363	19.4	67
97	Monolayer SnP: an excellent p-type thermoelectric material. *Nanoscale*, **2019**, 11, 19923-19932	7.7	66
96	Phonon spectrum, thermodynamic properties, and pressure-temperature phase diagram of uranium dioxide. *Physical Review B*, **2013**, 88,	3.3	57
95	First-principles study of ground-state properties and high pressure behavior of ThO2. *Journal of Nuclear Materials*, **2010**, 399, 181-188	3.3	54
94	First-principles LDA+U and GGA+U study of neptunium dioxide. *Physical Review B*, **2010**, 81,	3.3	52
93	Understanding the Effect of Local Short-Range Ordering on Lithium Diffusion in Li1.3Nb0.3Mn0.4O2 Single-Crystal Cathode. *CheM*, **2018**, 4, 2108-2123	16.2	50
92	First-principles calculations of phase transition, elastic modulus, and superconductivity under pressure for zirconium. *Journal of Applied Physics*, **2011**, 109, 063514	2.5	50
91	Hexagonal TiB monolayer: a promising anode material offering high rate capability for Li-ion and Na-ion batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 22168-22178	3.6	49
90	First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. *Physical Review B*, **2018**, 98,	3.3	48
89	Tetragonal and trigonal MoB monolayers: two new low-dimensional materials for Li-ion and Na-ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 5178-5188	3.6	45
88	First-principles study of ground state properties of ZrH2. *Computational Materials Science*, **2011**, 50, 3297-3302	3.3	40
87	RGO induced one-dimensional bimetallic carbide nanorods: An efficient and pH-universal hydrogen evolution reaction electrocatalyst. *Nano Energy*, **2019**, 62, 85-93	17.1	37
86	Monolayer Zr2B2: A promising two-dimensional anode material for Li-ion batteries. *Applied Surface Science*, **2019**, 480, 448-453	6.7	37
85	Electronic structures and mechanical properties of uranium monocarbide from first-principles LDA+U and GGA+U calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 3577-3581	2.3	35
84	A new 2D monolayer BiXene, M2C (M = Mo, Tc, Os). *Nanoscale*, **2016**, 8, 15753-62	7.7	35
83	Phonon spectrum and bonding properties of Bi2Se3: Role of strong spin-orbit interaction. *Applied Physics Letters*, **2012**, 100, 082109	3.4	32

82	Electronic structures, mechanical and thermodynamic properties of ThN from first-principles calculations. *Journal of Nuclear Materials*, **2011**, 408, 136-141	3.3	30
81	Hexagonal M2C3 (M = As, Sb, and Bi) monolayers: new functional materials with desirable band gaps and ultrahigh carrier mobility. *Journal of Materials Chemistry C*, **2018**, 6, 12689-12697	7.1	30
80	Prediction of phonon-mediated superconductivity in two-dimensional Mo2B2. *Journal of Materials Chemistry C*, **2019**, 7, 2589-2595	7.1	29
79	Evolution of Local Structural Ordering and Chemical Distribution upon Delithiation of a Rock Salt□tructured Li1.3Ta0.3Mn0.4O2 Cathode. *Advanced Functional Materials*, **2019**, 29, 1808294	15.6	29
78	First-principles calculations of phase transition, elasticity, and thermodynamic properties for TiZr alloy. *Journal of Nuclear Materials*, **2012**, 420, 501-507	3.3	29
77	Structural, electronic, and thermodynamic properties of UN: Systematic density functional calculations. *Journal of Nuclear Materials*, **2010**, 406, 218-222	3.3	29
76	Electronic and mechanical properties of ordered (Pu, U) O2 compounds: A density functional theory +U study. *Journal of Nuclear Materials*, **2013**, 433, 345-350	3.3	28
75	First-principles study of thermal transport properties in the two- and three-dimensional forms of BiOSe. *Physical Chemistry Chemical Physics*, **2019**, 21, 10931-10938	3.6	27
74	Ultralow thermal conductivity from transverse acoustic phonon suppression in distorted crystalline □MgAgSb. *Nature Communications*, **2020**, 11, 942	17.4	26
73	Superconductivity in two-dimensional phosphorus carbide (□PC). *Physical Chemistry Chemical Physics*, **2018**, 20, 12362-12367	3.6	26
72	High Thermoelectric Performance of New Two-Dimensional IV□VI Compounds: A First-Principles Study. *Journal of Physical Chemistry C*, **2020**, 124, 1812-1819	3.8	25
71	Electronic, mechanical, and thermodynamic properties of americium dioxide. *Journal of Nuclear Materials*, **2013**, 441, 411-420	3.3	24
70	Solution and diffusion of hydrogen isotopes in tungsten-rhenium alloy. *Journal of Nuclear Materials*, **2017**, 491, 206-212	3.3	22
69	Structural, electronic, and thermodynamic properties of curium dioxide: Density functional theory calculations. *Physical Review B*, **2017**, 96,	3.3	22
68	KAgX (X = S, Se): High-Performance Layered Thermoelectric Materials for Medium-Temperature Applications. *ACS Applied Materials & Interfaces*, **2020**, 12, 36102-36109	9.5	22
67	First-principles calculations of thermal transport properties in MoS/MoSe bilayer heterostructure. *Physical Chemistry Chemical Physics*, **2019**, 21, 10442-10448	3.6	21
66	Structural, electronic, mechanical, and thermodynamic properties of UN2: Systematic density functional calculations. *Journal of Nuclear Materials*, **2011**, 410, 46-51	3.3	21
65	Mechanical and chemical bonding properties of ground state BeH2. *European Physical Journal B*, **2010**, 74, 303-308	1.2	20

64	Lattice dynamics and chemical bonding in Sb2Te3 from first-principles calculations. *Journal of Chemical Physics*, **2015**, 142, 174702	3.9	19
63	Thermal conductivity of UO2 and PuO2 from first-principles. *Journal of Alloys and Compounds*, **2015**, 628, 267-271	5.7	19
62	Structural, mechanical, thermodynamic, and electronic properties of thorium hydrides from first-principles. *Journal of Nuclear Materials*, **2010**, 401, 124-129	3.3	19
61	Electronic transport properties of selected carbon □bowls with different size, curvature and solid state packing. *Carbon*, **2015**, 94, 174-180	10.4	18
60	First-principles study of UC2 and U2C3. *Journal of Nuclear Materials*, **2010**, 396, 218-222	3.3	18
59	Theoretical dissection of superconductivity in two-dimensional honeycomb borophene oxide B2O crystal with a high stability. *Npj Computational Materials*, **2020**, 6,	10.9	18
58	Electronic, mechanical and thermodynamic properties of □UH3: A comparative study by using the LDA and LDA+U approaches. *Journal of Nuclear Materials*, **2012**, 430, 137-141	3.3	17
57	Superconductivity in predicted two dimensional XB6 (X = Ga, In). *Journal of Materials Chemistry C*, **2020**, 8, 1704-1714	7.1	17
56	Thermoelectric Properties of Hexagonal M□□(M = As, Sb, and Bi) Monolayers from First-Principles Calculations. *Nanomaterials*, **2019**, 9,	5.4	16
55	Electronic structure and phase stability of plutonium hydrides: Role of Coulomb repulsion and spin-orbital coupling. *International Journal of Hydrogen Energy*, **2014**, 39, 13255-13265	6.7	16
54	Molecular dynamics simulations of hcp/fcc nucleation and growth in bcc iron driven by uniaxial compression. *Journal of Physics Condensed Matter*, **2009**, 21, 495702	1.8	16
53	Nucleation of hcp and fcc phases in bcc iron under uniform compression: classical molecular dynamics simulations. *Journal of Physics Condensed Matter*, **2010**, 22, 435404	1.8	15
52	Two-dimensional tetragonal Ti2BN: A novel potential anode material for Li-ion batteries. *Applied Surface Science*, **2020**, 513, 145821	6.7	14
51	Novel two-dimensional tetragonal vanadium carbides and nitrides as promising materials for Li-ion batteries. *Physical Chemistry Chemical Physics*, **2019**, 21, 19513-19520	3.6	14
50	Emergence of superconductivity in a Dirac nodal-line Cu2Si monolayer: ab initio calculations. *Journal of Materials Chemistry C*, **2019**, 7, 10926-10932	7.1	13
49	First-principles study of pressure-induced phase transition and electronic property of PbCrO3. *Journal of Applied Physics*, **2012**, 111, 013503	2.5	13
48	Novel structures of two-dimensional tungsten boride and their superconductivity. *Physical Chemistry Chemical Physics*, **2019**, 21, 15327-15338	3.6	12
47	First-principles study of superconductivity in the two- and three-dimensional forms of PbTiSe2: Suppressed charge density wave in 1T□iSe2. *Physical Review B*, **2018**, 98,	3.3	12

46	Imaging and spectrum of monolayer graphene oxide in external electric field. *Carbon*, **2015**, 93, 843-850	10.4	11
45	First-principles calculations of phase transition, elasticity, phonon spectra, and thermodynamic properties for hafnium. *Computational Materials Science*, **2019**, 157, 121-131	3.2	11
44	Cone-spiral magnetic ordering dominated lattice distortion and giant negative thermal expansion in Fe-doped MnNiGe compounds. *Materials Horizons*, **2020**, 7, 804-810	14.4	9
43	Face-centered cubic MoS2: a novel superconducting three-dimensional crystal more stable than layered T-MoS2. *Journal of Materials Chemistry C*, **2018**, 6, 6046-6051	7.1	8
42	Evolution of the topologically protected surface states in superconductor BiPd from the three-dimensional to the two-dimensional limit. *Journal of Physics Condensed Matter*, **2017**, 29, 325501	1.8	8
41	Topological and superconducting properties in YD3 (D=In, Sn, Tl, Pb). *Physical Review Materials*, **2019**, 3,	3.2	8
40	Thermal transport properties of monolayer MoSe with defects. *Physical Chemistry Chemical Physics*, **2020**, 22, 5832-5838	3.6	8
39	Mechanical and thermodynamic properties of plutonium dihydride. *Journal of Alloys and Compounds*, **2018**, 750, 258-264	5.7	7
38	Mechanics, Lattice Dynamics, and Chemical Bonding in ZrB2 and ZrB12 from First-Principles Calculations. *Science of Advanced Materials*, **2013**, 5, 1916-1921	2.3	7
37	Nonhelical spin texture in the normal states of the centrosymmetric superconductor RdBi2. *Physical Review B*, **2019**, 100,	3.3	6
36	Lattice vibrational modes and phonon thermal conductivity of single-layer GaGeTe. *Journal of Materiomics*, **2020**, 6, 723-728	6.7	6
35	Significant enhancement of the thermoelectric properties of CaP3 through reducing the dimensionality. *Materials Advances*, **2020**, 1, 3322-3332	3.3	6
34	First-principles prediction of ideal type-II Weyl phonons in wurtzite ZnSe. *Physical Review B*, **2021**, 103,	3.3	6
33	Quadruple-layer group-IV tellurides: low thermal conductivity and high performance two-dimensional thermoelectric materials. *Physical Chemistry Chemical Physics*, **2021**, 23, 6388-6396	3.6	6
32	Square transition-metal carbides MC (M = Mo, W) as stable two-dimensional Dirac cone materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 732-737	3.6	6
31	Observing and tuning the density distribution of localized states of monolayer graphene oxide by using external electric field. *Applied Physics Letters*, **2015**, 106, 131103	3.4	5
30	Temperature-driven stabilization of fcc-ThH2 from first-principles theory coupled with lattice dynamics. *Computational Materials Science*, **2015**, 98, 15-17	3.2	5
29	First principles calculations on the thermoelectric properties of bulk Au2S with ultra-low lattice thermal conductivity. *Chinese Physics B*, **2020**, 29, 087202	1.2	5

28	Electron-phonon coupling superconductivity in two-dimensional orthorhombic MB6 (M=Mg,Ca,Ti,Y) and hexagonal MB6 (M=Mg,Ca,Sc,Ti). *Physical Review Materials*, **2020**, 4,	3.2	5
27	YS2 monolayer as a high-efficient anode material for rechargeable Li-ion and Na-ion batteries. *Solid State Ionics*, **2020**, 345, 115187	3.3	5
26	Understanding of transition metal (Ru, W) doping into Nb for improved thermodynamic stability and hydrogen permeability: density functional theory calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 17538-17545	3.6	4
25	Prediction of superconductivity and topological aspects in single-layer Bi2Pd. *Physical Review B*, **2020**, 102,	3.3	4
24	Physical design of multipurpose physics neutron diffractometer for the CSNS. *Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **2019**, 927, 161-168	1.2	4
23	Structural, electronic, and elastic properties of equiatomic UZr alloys from first-principles. *Journal of Nuclear Materials*, **2017**, 496, 333-342	3.3	3
22	Ideal Strengths and Bonding Properties of PuO 2 under Tension. *Chinese Physics Letters*, **2011**, 28, 047101	1.8	3
21	Charge density wave and pressure-dependent superconductivity in the kagome metal CsV3Sb5 : A first-principles study. *Physical Review B*, **2022**, 105,	3.3	3
20	Surface passivation induced a significant enhancement of superconductivity in layered two-dimensional MSiN (M = Ta and Nb) materials. *Nanoscale*, **2021**, 13, 18947-18954	7.7	3
19	Single-Layer Dititanium Oxide TiO MOene: Multifunctional Promises for Electride, Anode Materials, and Superconductor. *Journal of Physical Chemistry Letters*, **2021**, 12, 494-500	6.4	3
18	Ideal Strengths and Bonding Properties of UO 2 under Tension. *Chinese Physics Letters*, **2015**, 32, 037102	1.8	2
17	Thermoelectric Properties of Hexagonal WN from First-Principles Calculations. *ES Energy & Environments*, **2018**,	2.9	2
16	Effect of Ni2+ on Lithium-Ion Diffusion in Layered LiNi1□MnxCoyO2 Materials. *Crystals*, **2021**, 11, 465	2.3	2
15	Pushing the limit of thermal conductivity of MAX borides and MABs. *Journal of Materials Science and Technology*, **2021**, 97, 79-79	9.1	2
14	Phase transition, elasticity, phonon spectra, and superconductive properties of equiatomic TiZr, TiHf, and ZrHf alloys at high pressure: Ab initio calculations. *Computational Materials Science*, **2020**, 178, 109637	3.2	2
13	Theoretical investigation of Ti2B monolayer as powerful anode material for Li/Na batteries with high storage capacity. *Applied Surface Science*, **2021**, 538, 148048	6.7	2
12	Black potassium titanate nanobelts: Ultrafast and durable aqueous redox electrolyte energy storage. *Journal of Power Sources*, **2021**, 483, 229140	8.9	2
11	Effects of pressure on structural, electronic, and mechanical properties of □ and □uranium. *Chinese Physics B*, **2017**, 26, 066104	1.2	1

10	Inelastic Electron Tunneling in 2H-Ta_{x}Nb_{1-x}Se_{2} Evidenced by Scanning Tunneling Spectroscopy. *Physical Review Letters*, **2020**, 124, 106403	7.4	1
9	Structural and electronic properties of Y2CrS4 from first-principles study. *European Physical Journal B*, **2011**, 80, 307-310	1.2	1
8	Zintl Phase BaAgSb: Low Thermal Conductivity and High Performance Thermoelectric Material in Ab Initio Calculation. *Chinese Physics Letters*, **2021**, 38, 046301	1.8	1
7	Novel 2D PC 5 with a Dirac Cone and Edge-Size Dependence. *Physica Status Solidi - Rapid Research Letters*,2100203	2.5	1
6	Topological Superconductivity in Rashba Spin-Orbital Coupling Suppressed Monolayer □Bi2Pd. *Materials Today Physics*, **2022**, 100674	8	1
5	Prediction of superconductivity in bilayer borophenes.. *RSC Advances*, **2021**, 11, 40220-40227	3.7	0
4	Anomalous optical and electronic properties of dense sodium. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 4458-4464	2.3	
3	High-pressure elastic anisotropy and superconductivity of hafnium: A first-principles calculation*. *Chinese Physics B*, **2021**, 30, 056202	1.2	
2	First-principles study of electronic structure and superconductivity of PbTa2Se. *Materials Research Express*, **2019**, 6, 046001	1.7	
1	Octahedral rotation induced spin state and metal□nsulator transition in LaCoO3 films. *Journal of Magnetism and Magnetic Materials*, **2022**, 169318	2.8	