Wei-Bing Zhang

List of Publications by Year in Descending Order

53 papers	1,667 citations	21 h-index	40 g-index
59 ext. papers	1,971 ext. citations	4 avg, IF	4.98 L-index

#	Paper	IF	Citations
53	A Study of transition metal dichalcogenides/Chromium Trihalides vdW heterostructure based on band unfolding method. *Wuli Xuebao/Acta Physica Sinica*, **2022**,	0.6	
52	Strain and electric field dependent spin polarization in two-dimensional arsenene/CrI3 heterostructure. *Journal of Alloys and Compounds*, **2022**, 912, 165093	5.7	
51	Revealing the Underlying Mechanisms of the Stacking Order and Interlayer Magnetism of Bilayer CrBr3. *Journal of Physical Chemistry C*, **2021**, 125, 7314-7320	3.8	4
50	Engineering the ligand states by surface functionalization: a new way to enhance the ferromagnetism of CrI. *Nanoscale*, **2021**, 13, 4821-4827	7.7	0
49	Electronic Structure and Magnetic Anisotropy of Single-Layer Rare-Earth Oxybromide. *ACS Omega*, **2020**, 5, 14194-14201	3.9	7
48	Electronic structures and strain responses of group VA/VA two-dimensional van der waals heterostructures. *Vacuum*, **2020**, 176, 109296	3.7	11
47	Tunable strain effects on the electronic structures and mobility properties of InP/InAs lateral heterostructure. *Journal Physics D: Applied Physics*, **2020**, 53, 505108	3	1
46	Spin-dependent Schottky barriers and vacancy-induced spin-selective ohmic contacts in magnetic vdW heterostructures. *Physical Chemistry Chemical Physics*, **2020**, 22, 9460-9466	3.6	6
45	Achieving a direct band gap and high power conversion efficiency in an SbI/BiI type-II vdW heterostructure via interlayer compression and electric field application. *Physical Chemistry Chemical Physics*, **2019**, 21, 2619-2627	3.6	9
44	The enhanced ferromagnetism of single-layer CrX (X = Br and I) via van der Waals engineering. *Physical Chemistry Chemical Physics*, **2019**, 21, 11949-11955	3.6	14
43	Structural, elastic and electronic properties of typical NdMgT 4 (T = Co, Ni, Cu) alloys from ab initio calculation. *Physica B: Condensed Matter*, **2018**, 540, 38-42	2.8	2
42	AI3 (A = As, Sb) Single Layers and Their vdW Heterostructure for Photocatalysis and Solar Cell Applications. *Journal of Physical Chemistry C*, **2018**, 122, 7656-7663	3.8	25
41	Electronic structure, optical properties and band edges of layered MoO3: A first-principles investigation. *Computational Materials Science*, **2017**, 130, 242-248	3.2	47
40	Tailoring Anisotropic Li-Ion Transport Tunnels on Orthogonally Arranged Li-Rich Layered Oxide Nanoplates Toward High-Performance Li-Ion Batteries. *Nano Letters*, **2017**, 17, 1670-1677	11.5	99
39	High-Mobility Transport Anisotropy in Few-Layer MoO and Its Origin. *ACS Applied Materials & Interfaces*, **2017**, 9, 1702-1709	9.5	36
38	Stability and carrier mobility of organic-inorganic hybrid perovskite CHNHPbI in two-dimensional limit. *Journal of Chemical Physics*, **2017**, 147, 164703	3.9	11
37	Theoretical perspective of energy harvesting properties of atomically thin BiI3. *Journal of Materials Chemistry A*, **2016**, 4, 19086-19094	13	41

36	Atomic-Scale Mechanism on Nucleation and Growth of MoC Nanoparticles Revealed by in Situ Transmission Electron Microscopy. *Nano Letters*, **2016**, 16, 7875-7881	11.5	21
35	Direct TEM observations of growth mechanisms of two-dimensional MoS2 flakes. *Nature Communications*, **2016**, 7, 12206	17.4	147
34	Atomically thin binary V-V compound semiconductor: a first-principles study. *Journal of Materials Chemistry C*, **2016**, 4, 6581-6587	7.1	98
33	Bending rigidity of transition metal dichalcogenide monolayers from first-principles. *Journal Physics D: Applied Physics*, **2016**, 49, 185301	3	23
32	Tunable electronic properties of GeSe/phosphorene heterostructure from first-principles study. *Applied Physics Letters*, **2016**, 109, 103104	3.4	71
31	Helix-like structure formation of a semi-flexible chain confined in a cylinder channel. *Chinese Physics B*, **2016**, 25, 093601	1.2	1
30	Tuning metal–graphene interaction by non-metal intercalation: a case study of the graphene/oxygen/Ni (1 1 1) system. *Journal Physics D: Applied Physics*, **2015**, 48, 015308	3	7
29	Electronic structures and elastic properties of monolayer and bilayer transition metal dichalcogenides MX 2 (M = Mo, W; X = O, S, Se, Te): A comparative first-principles study. *Chinese Physics B*, **2015**, 24, 097103	1.2	66
28	First-Principle Calculations of the MgYA4 (A = Co and Ni) Phase with AuBe5-Type Structure. *Acta Metallurgica Sinica (English Letters)*, **2015**, 28, 1326-1331	2.5	1
27	Robust intrinsic ferromagnetism and half semiconductivity in stable two-dimensional single-layer chromium trihalides. *Journal of Materials Chemistry C*, **2015**, 3, 12457-12468	7.1	388
26	The tunable electronic structure and mechanical properties of halogenated silicene: a first-principles study. *Journal of Materials Chemistry C*, **2015**, 3, 3087-3094	7.1	47
25	Electronic structure and thermodynamic properties of millerite NiS from first principles: Complex fermi surface and large thermal expansion coefficient. *Computational Materials Science*, **2014**, 83, 412-417	3.2	12
24	First-principles study for stability and binding mechanism of graphene/Ni(111) interface: Role of vdW interaction. *Journal of Chemical Physics*, **2014**, 141, 044708	3.9	51
23	Tuning the crystal shape of materials by chemical potential: a combined theoretical and experimental study for NiSe2. *RSC Advances*, **2014**, 4, 13395-13404	3.7	2
22	Equilibrium Crystal Shape of Ni from First Principles. *Journal of Physical Chemistry C*, **2013**, 117, 21274-21280	4.8	40
21	Role of electronic correlation in high-low temperature phase transition of hexagonal nickel sulfide: a comparative density functional theory study with and without correction for on-site Coulomb interaction. *Journal of Chemical Physics*, **2013**, 138, 244703	3.9	10
20	A Comparative Density-Functional Theory Investigation of Oxygen Adsorption on Stepped Ni Surfaces 3(hkl)[111) [hkl=(111),(100),(110)]: Role of Terrace Orientation. *Journal of the Physical Society of Japan*, **2013**, 82, 074709	1.5	4
19	Elastic and electronic properties of a new MAX compound (Cr0.5V0.5)2GeC from first-principles calculations. *Solid State Communications*, **2010**, 150, 49-53	1.6	16

18	Oxygen adsorption on stepped Pd(100) surfaces. *Surface Science*, **2010**, 604, 1813-1819	1.8	14
17	Surface adsorption phase diagram of O/Ni(110) system: An ab initio atomistic thermodynamics investigation. *Applied Physics Letters*, **2009**, 94, 091901	3.4	4
16	First-principles studies of the oxygen adsorption on unreconstructed and reconstructed Ni(1 1 0) surfaces. *Surface Science*, **2009**, 603, 1002-1009	1.8	12
15	Energetics and electronic properties of Mg7TMH16 (TM=Sc, Ti, V, Y, Zr, Nb): An ab initio study. *Physica B: Condensed Matter*, **2009**, 404, 2234-2240	2.8	34
14	Stability of MgO(111) Polar Surface: Effect of the Environment. *Journal of Physical Chemistry C*, **2008**, 112, 3327-3333	3.8	21
13	Initial stage of Ag deposition on regular MgO(001) surface: A DFT study. *Computational Materials Science*, **2008**, 42, 43-49	3.2	15
12	Crystal structure of Mg3Pd from first-principles calculations. *Transactions of Nonferrous Metals Society of China*, **2008**, 18, 416-420	3.3	10
11	Water Adsorption on a NiO(100) Surface: A GGA+U Study. *Journal of Physical Chemistry C*, **2008**, 112, 452-457	3.8	36
10	Stability of the polar NiO(111) surface. *Journal of Chemical Physics*, **2008**, 128, 124703	3.9	33
9	Adsorption of oxygen atoms on the Mg3Nd(001) surface. *Journal of Applied Physics*, **2008**, 104, 033516	2.5	
8	Electronic structure and Fermi surface character of LaNiPO from first principles. *Physical Review B*, **2008**, 77,	3.3	19
7	Stability and magnetism of vacancy in NiO: A GGA+U study. *European Physical Journal B*, **2008**, 64, 153-158	1.2	45
6	First-principles study of structural stabilities and electronic characteristics of Mg□a intermetallic compounds. *Computational Materials Science*, **2007**, 41, 78-85	3.2	40
5	Structural distortion of -structured MnO and FeO. *Solid State Communications*, **2007**, 142, 6-9	1.6	18
4	Pressure dependence of exchange interactions in NiO. *Physical Review B*, **2006**, 74,	3.3	34
3	Structural distortion and electronic properties of NiO under high pressure: anab initioGGA+Ustudy. *Journal of Physics Condensed Matter*, **2006**, 18, 9691-9701	1.8	8
2	Phase stability and structural distortion of NiO under high pressure. *Transactions of Nonferrous Metals Society of China*, **2006**, 16, s52-s58	3.3	2
1	Adsorption of atomic S and C on Mg(0001) surface. *Transactions of Nonferrous Metals Society of China*, **2006**, 16, s253-s256	3.3	1