Wei-Bing Zhang

List of Publications by Year
in descending order

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58 papers	2,218 citations	279487 23 h-index	214527 47 g-index
59 all docs	59 docs citations	59 times ranked	4061 citing authors

#	Article	IF	Citations
1	Robust intrinsic ferromagnetism and half semiconductivity in stable two-dimensional single-layer chromium trihalides. Journal of Materials Chemistry C, 2015, 3, 12457-12468.	2.7	569
2	Direct TEM observations of growth mechanisms of two-dimensional MoS2 flakes. Nature Communications, 2016, 7, 12206.	5.8	179
3	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.	4.5	128
4	Atomically thin binary Vâ€“V compound semiconductor: a first-principles study. Journal of Materials Chemistry C, 2016, 4, 6581-6587.	2.7	126
5	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.	0.7	98
6	Tunable electronic properties of GeSe/phosphorene heterostructure from first-principles study. Applied Physics Letters, 2016, 109, .	1.5	87
7	Electronic structure, optical properties and band edges of layered MoO3: A first-principles investigation. Computational Materials Science, 2017, 130, 242-248.	1.4	76
8	Equilibrium Crystal Shape of Ni from First Principles. Journal of Physical Chemistry C, 2013, 117, 21274-21280.	1.5	60
9	Stability and magnetism of vacancy in NiO: A GGA+U study. European Physical Journal B, 2008, 64, 153-158.	0.6	57
10	First-principles study for stability and binding mechanism of graphene/Ni(111) interface: Role of vdW interaction. Journal of Chemical Physics, 2014, 141, 044708.	1.2	56
11	The tunable electronic structure and mechanical properties of halogenated silicene: a first-principles study. Journal of Materials Chemistry C, 2015, 3, 3087-3094.	2.7	54
12	High-Mobility Transport Anisotropy in Few-Layer MoO₃ and Its Origin. ACS Applied Materials & Interfaces, 2017, 9, 1702-1709.	4.0	51
13	Theoretical perspective of energy harvesting properties of atomically thin BiI₃. Journal of Materials Chemistry A, 2016, 4, 19086-19094.	5.2	47
14	Water Adsorption on a NiO(100) Surface:â€‰ A GGA+U Study. Journal of Physical Chemistry C, 2008, 112, 452-457.	1.5	43
15	First-principles study of structural stabilities and electronic characteristics of Mgâ€“La intermetallic compounds. Computational Materials Science, 2007, 41, 78-85.	1.4	42
16	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.	1.3	42
17	Stability of the polar NiO(111) surface. Journal of Chemical Physics, 2008, 128, 124703.	1.2	41
18	Pressure dependence of exchange interactions inNiO. Physical Review B, 2006, 74, .	1.1	39

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19	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.	1.5	34
20	Bending rigidity of transition metal dichalcogenide monolayers from first-principles. Journal Physics D: Applied Physics, 2016, 49, 185301.	1.3	33
21	Atomic-Scale Mechanism on Nucleation and Growth of Mo₂C Nanoparticles Revealed by in Situ Transmission Electron Microscopy. Nano Letters, 2016, 16, 7875-7881.	4.5	28
22	Stability of MgO(111) Polar Surface:â€‰ Effect of the Environment. Journal of Physical Chemistry C, 2008, 112, 3327-3333.	1.5	26
23	The enhanced ferromagnetism of single-layer CrX₃ (X = Br and I) via van der Waals engineering. Physical Chemistry Chemical Physics, 2019, 21, 11949-11955.	1.3	26
24	Structural distortion of -structured MnO and FeO. Solid State Communications, 2007, 142, 6-9.	0.9	19
25	Electronic structure and Fermi surface character of LaNiPO from first principles. Physical Review B, 2008, 77, .	1.1	19
26	Elastic and electronic properties of a new MAX compound from first-principles calculations. Solid State Communications, 2010, 150, 49-53.	0.9	18
27	Oxygen adsorption on stepped Pd(100) surfaces. Surface Science, 2010, 604, 1813-1819.	0.8	18
28	Stability and carrier mobility of organic-inorganic hybrid perovskite CH3NH3PbI3 in two-dimensional limit. Journal of Chemical Physics, 2017, 147, 164703.	1.2	16
29	Revealing the Underlying Mechanisms of the Stacking Order and Interlayer Magnetism of Bilayer CrBr₃. Journal of Physical Chemistry C, 2021, 125, 7314-7320.	1.5	16
30	Initial stage of Ag deposition on regular MgO(001) surface: A DFT study. Computational Materials Science, 2008, 42, 43-49.	1.4	15
31	Spin-dependent Schottky barriers and vacancy-induced spin-selective ohmic contacts in magnetic vdW heterostructures. Physical Chemistry Chemical Physics, 2020, 22, 9460-9466.	1.3	14
32	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.	1.2	13
33	Achieving a direct band gap and high power conversion efficiency in an SbI₃/BiI₃ type-II vdW heterostructure via interlayer compression and electric field application. Physical Chemistry Chemical Physics, 2019, 21, 2619-2627.	1.3	13
34	First-principles studies of the oxygen adsorption on unreconstructed and reconstructed Ni(110) surfaces. Surface Science, 2009, 603, 1002-1009.	0.8	12
35	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.	1.4	12
36	Electronic structures and strain responses of group VA/VA two-dimensional van der waals heterostructures. Vacuum, 2020, 176, 109296.	1.6	12

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37	Crystal structure of Mg3Pd from first-principles calculations. Transactions of Nonferrous Metals Society of China, 2008, 18, 416-420.	1.7	10
38	Electronic Structure and Magnetic Anisotropy of Single-Layer Rare-Earth Oxybromide. ACS Omega, 2020, 5, 14194-14201.	1.6	10
39	Structural distortion and electronic properties of NiO under high pressure: anab initioGGA+Ustudy. Journal of Physics Condensed Matter, 2006, 18, 9691-9701.	0.7	8
40	Tuning metalâ€“graphene interaction by non-metal intercalation: a case study of the graphene/oxygen/Ni (1â€‰×â€‰1) system. Journal Physics D: Applied Physics, 2015, 48, 015308.	1.3	8
41	Eï¬€ect of Thickness and Stacking Order on Raman Spectrum of Layered CrCl3. Journal of Physics Condensed Matter, 2021, 33, .	0.7	5
42	Surface adsorption phase diagram of O/Ni(110) system: An ab initio atomistic thermodynamics investigation. Applied Physics Letters, 2009, 94, 091901.	1.5	4
43	A Comparative Density-Functional Theory Investigation of Oxygen Adsorption on Stepped Ni Surfaces 3(hkl)Ã—(111) [hkl=(111),(100),(110)]: Role of Terrace Orientation. Journal of the Physical Society of Japan, 2013, 82, 074709.	0.7	4
44	Tuning the crystal shape of materials by chemical potential: a combined theoretical and experimental study for NiSe2. RSC Advances, 2014, 4, 13395-13404.	1.7	4
45	First-Principle Calculations of the MgYA4 (AÂ=ÂCo and Ni) Phase with AuBe5-Type Structure. Acta Metallurgica Sinica (English Letters), 2015, 28, 1326-1331.	1.5	4
46	A simple descriptor for magnetic classification of 2D MXene materials. AIP Advances, 2022, 12, .	0.6	4
47	Structural, elastic and electronic properties of typical NdMgT 4 (Tâ€¯=â€¯Co, Ni, Cu) alloys from ab initio calculation. Physica B: Condensed Matter, 2018, 540, 38-42.	1.3	3
48	Engineering the ligand states by surface functionalization: a new way to enhance the ferromagnetism of CrI₃. Nanoscale, 2021, 13, 4821-4827.	2.8	3
49	Giant interlayer magnetic exchange interaction and charge-spin coupling in a van der Waals magnetic interface driven by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi><mml:mo>â^'</mml:mo><mml:mi>d</mml:mi></mml:ma coupling. Physical Review B, 2022, 105, .	1.1	3
50	Phase stability and structural distortion of NiO under high pressure. Transactions of Nonferrous Metals Society of China, 2006, 16, s52-s58.	1.7	2
51	Tunable strain effects on the electronic structures and mobility properties of InP/InAs lateral heterostructure. Journal Physics D: Applied Physics, 2020, 53, 505108.	1.3	2
52	Adsorption of atomic S and C on Mg(0001) surface. Transactions of Nonferrous Metals Society of China, 2006, 16, s253-s256.	1.7	1
53	Helix-like structure formation of a semi-flexible chain confined in a cylinder channel. Chinese Physics B, 2016, 25, 093601.	0.7	1
54	Strain and electric field dependent spin polarization in two-dimensional arsenene/CrI3 heterostructure. Journal of Alloys and Compounds, 2022, 912, 165093.	2.8	1

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55	Adsorption of oxygen atoms on the Mg3Nd(001) surface. Journal of Applied Physics, 2008, 104, 033516.	1.1	0
56	Raman Spectrum of layered Ferromagnetic Material VI3 from First-principles. , 2021, , .		0
57	å±‚çŠ¶3d²ä½“ç³»VI₃çš„æ™¶ä½“ç»“æž„å’Œ Physica, Mechanica Et Astronomica, 2022, , .	0.2	0
58	A Study of transition metal dichalcogenides/Chromium Trihalides vdW heterostructure based on band unfolding method. Wuli Xuebao/Acta Physica Sinica, 2022, .	0.2	0