Kaihua He

List of Publications by Year
in descending order

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39	381	687335	794568
papers	citations	13 h-index	19 g-index

39	39	39	548
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First principles study of the lattice thermal conductivity of alkaline earth oxides. Computational Materials Science, 2022, 210, 111446.	3.0	4
2	Influence of Cu dopant on the electronic and optical properties of graphene-like ZnO monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 115, 113702.	2.7	16
3	Theoretical investigations on the structural stability, structural and physical properties, and bonding feature for RuX (X = Si, Ge, Sn) with B20 and B2 phases. Materials Today Communications, 2020, 24, 101116.	1.9	2
4	Structural, elastic, electronic and optical properties of lithium halides (LiF, LiCl, LiBr, and LiI): First-principle calculations. Materials Chemistry and Physics, 2020, 244, 122733.	4.0	22
5	First principles studied tunable electronic and optical properties of 2D honeycomb ZnO monolayer engineered by biaxial strain and intrinsic vacancy. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2020, 254, 114517.	3.5	15
6	First-principles study on the electronic and optical properties of two-dimensional graphene-like Zn1â^'xVxO (xâ€¯=â€¯0.0625, 0.125) monolayer. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 113, 143-151.	2.7	4
7	Effects of iron spin transition on the electronic structure, thermal expansivity and lattice thermal conductivity of ferropericlase: a first principles study. Scientific Reports, 2019, 9, 4172.	3.3	10
8	The thermodynamic, electronic and optical properties of GeP type ZnO under pressure calculated by Debye model and hybrid function. Materials Chemistry and Physics, 2018, 211, 206-213.	4.0	2
9	First principles and Debye model study of the thermodynamic, electronic and optical properties of MgO under high-temperature and pressure. International Journal of Modern Physics B, 2018, 32, 1850047.	2.0	0
10	Structure, electric, elastic and optical properties of Mn2+-doped MgAl2O4 spinel with/without an O-vacancy. Physica B: Condensed Matter, 2018, 547, 111-119.	2.7	3
11	The effect of the Zn/Sn ratio on the formation of single phase kesterite Cu 2 ZnSnS 4 solar cell material. Ceramics International, 2017, 43, 8103-8108.	4.8	10
12	The GGA+U method studied the effects of Cu doping on the formation energy, electronic and optical properties of V-doped ZnO. Optical and Quantum Electronics, 2017, 49, 1.	3.3	3
13	First principles study of the Mn-doping effect on the physical and chemical properties of mullite-family Al₂SiO₅. Physical Chemistry Chemical Physics, 2017, 19, 24991-25001.	2.8	5
14	Mechanisms of Incorporation of Hydroxyl in Coesite. Journal of Nanoscience and Nanotechnology, 2017, 17, 6716-6720.	0.9	1
15	Transmission Electron Microscopy Analysis and First-Principles Calculations of Phase Transition from Coesite to Quartz. Journal of Nanoscience and Nanotechnology, 2017, 17, 6754-6758.	0.9	0
16	Water Contents and Vacancies of Zircon: Insight from Fourier Transform Infrared Spectroscopy and First Principles Calculation. Journal of Nanoscience and Nanotechnology, 2017, 17, 6470-6481.	0.9	0
17	Two-Dimensional Ordering of Ionic Liquids Confined by Layered Silicate Plates via Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2015, 119, 19244-19252.	3.1	27
18	GGA+U study of the electronic and optical properties of hexagonal BN phase ZnO under pressure. Computational Materials Science, 2015, 102, 196-201.	3.0	20

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19	First-principles study of spin transition and seismic properties of ferric iron-bearing post-perovskite with oxygen vacancy. Physics and Chemistry of Minerals, 2015, 42, 163-169.	0.8	0
20	Electronic Structures of S/C-Doped TiO₂Anatase (101) Surface: First-Principles Calculations. International Journal of Photoenergy, 2014, 2014, 1-7.	2.5	1
21	Ultra-thin L10-FePt for perpendicular anisotropy L10-FePt/Ag/[Co/Pd]30 pseudo spin valves. Journal of Applied Physics, 2014, 115, 17C102.	2.5	4
22	The optical properties of NiAs phase ZnO under pressure calculated by GGA+U method. Optics Communications, 2014, 312, 185-191.	2.1	23
23	First principles study of magnetic anisotropy and magnetoelectric effect of FePd/MgO(001) ultrathin films. Journal of Applied Physics, 2013, 113, .	2.5	8
24	Effect of oxygen vacancies on the electronic structure and transport properties of SrRuO3 thin films. Journal of Applied Physics, 2013, 113, .	2.5	19
25	First-principles study of hydrogen adsorption on titanium-decorated single-layer and bilayer graphenes. Chinese Physics B, 2013, 22, 067101.	1.4	14
26	The role of octahedral tilting in the structural phase transition and magnetic anisotropy in SrRuO3 thin film. Journal of Applied Physics, 2013, 113, .	2.5	40
27	FIRST-PRINCIPLES CALCULATIONS ON ELECTRONIC STRUCTURES OF TiO2 ANATASE (101) SURFACES WITH N IMPURITIES. Modern Physics Letters B, 2011, 25, 119-129.	1.9	4
28	REACTIVITY AND STABILITY OF OXYGEN VACANCIES ON TiO₂ ANATASE (101) SURFACE: FIRST-PRINCIPLES CALCULATIONS. International Journal of Modern Physics B, 2011, 25, 4029-4037.	2.0	1
29	First-principles study on adsorption of Au atom on hydroxylated SiO2 surface. Journal Wuhan University of Technology, Materials Science Edition, 2011, 26, 1184-1188.	1.0	3
30	First-principles calculations on electronic structures of Fe-vacancy-codoped TiO2 anatase (101) surface. Physica B: Condensed Matter, 2011, 406, 3841-3846.	2.7	29
31	First principles study on the electronic structure and effect of vanadium doping of BN nanowires. Solid State Communications, 2010, 150, 701-706.	1.9	11
32	COMPARATIVE STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF BN(5, 5) AND C(5, 5) NANOTUBES UNDER PRESSURE. International Journal of Modern Physics B, 2010, 24, 4851-4859.	2.0	1
33	FIRST-PRINCIPLES STUDY OF THE EFFECTS OF THE OXYGEN VACANCY ON ELECTRONIC STRUCTURE AND FERROMAGNETISM OF Sn₂Co₂O_{8-Î´}. International Journal of Modern Physics B, 2010, 24, 2229-2235.	2.0	1
34	Asymmetric Fabryâ€“PÃ©rot fiber-optic pressure sensor for liquid-level measurement. Review of Scientific Instruments, 2009, 80, 033104.	1.3	20
35	The electronic structure and ferromagnetism of TM (TM=V, Cr, and Mn)-doped BN(5,5) nanotube: A first-principles study. Physica B: Condensed Matter, 2008, 403, 4213-4216.	2.7	26
36	FIRST PRINCIPLES STUDY OF THE ELECTRONIC STRUCTURE AND FERROMAGNETISM OF THE V-DOPED BN(5, 5) NANOTUBE. Modern Physics Letters B, 2008, 22, 1749-1756.	1.9	6

#	Article	IF	Citations
37	Effects of single oxygen vacancy on electronic structure and ferromagnetism for V-doped TiO2. Solid State Communications, 2007, 144, 54-57.	1.9	21
38	Ab initio study of structural, electronic and optical properties of MnHg(SCN)4 and FeHg(SCN)4. Physica B: Condensed Matter, 2007, 390, 231-235.	2.7	5
39	First-principles calculations of the exchange coupling constants in. Journal of Magnetism and Magnetic Materials, 2007, 310, e264-e265.	2.3	0