Xiao-Chun Wang

List of Publications by Year
in descending order

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35 papers	576 citations	623574 14 h-index	642610 23 g-index
35 all docs	35 docs citations	35 times ranked	500 citing authors

#	Article	IF	Citations
1	The adsorption characteristics of CO, NO and NO2 on two dimensional metalloporphyrin porous nanosheets: A first-principles study. Applied Surface Science, 2022, 582, 152469.	3.1	9
2	Enhanced thermoelectric performance based on special micro-configuration of graphene-ZnO induced by high-pressure and high-temperature. Ceramics International, 2022, 48, 9014-9023.	2.3	5
3	The flexible Janus X2PAs (XÂ=ÂSi, Ge and Sn) monolayers with in-plane and out-of-plane piezoelectricity. Applied Surface Science, 2022, 589, 152999.	3.1	23
4	Essential effect of proton coupled electron sequent transfer on photocatalytic water complete dissociation: A DFT study. International Journal of Hydrogen Energy, 2021, 46, 34216-34228.	3.8	5
5	Electron reservoir enhances methane conversion on Zn dimer supported by N doped graphene: A DFT study. Applied Surface Science, 2021, 563, 150328.	3.1	4
6	Electronic properties of double-atom catalysts for electrocatalytic oxygen evolution reaction in alkaline solution: a DFT study. Nanoscale, 2021, 14, 187-195.	2.8	17
7	Enhanced out-of-plane piezoelectricity of group-III(A) Janus hydrofluoride monolayers. Physical Review B, 2021, 104, .	1.1	17
8	Janus structure derivatives SnPâ€“InS, GeP-GaS and SiPâ€“AlS monolayers with in-plane and out-of-plane piezoelectric performance. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113817.	1.3	12
9	New direction's piezoelectricity and new applications of two-dimensional group V-IV-III-VI films: A theoretical study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114214.	1.3	9
10	The sustainable cyclic process of water molecule dissociation on the boron-functionalized graphene monovacancy: First-principles study. Applied Surface Science, 2019, 498, 143823.	3.1	13
11	Photoelectron imaging of resonance-enhanced multiphoton ionization and above-threshold ionization of ammonia molecules in a strong 800-nm laser pulse*. Chinese Physics B, 2019, 28, 063201.	0.7	6
12	DFT study on the oxygen titanium porphyrin as sustainable cyclic catalyst for water splitting. International Journal of Hydrogen Energy, 2019, 44, 19920-19928.	3.8	15
13	Imaging alignment of rotational state-selected CH 3 I molecule. Chinese Physics B, 2019, 28, 023101.	0.7	2
14	Piezoelectricity and dipolar polarization of group V-IV-III-VI sheets: A first-principles study. Applied Surface Science, 2019, 463, 918-922.	3.1	15
15	Magnetism and piezoelectricity of hexagonal boron nitride with triangular vacancy. Chinese Physics B, 2018, 27, 016301.	0.7	13
16	Piezoelectric and polarized enhancement by hydrofluorination of penta-graphene. Physical Chemistry Chemical Physics, 2018, 20, 26288-26296.	1.3	26
17	Tuning the electronic and magnetic property of semihydrogenated graphene and monolayer boron nitride heterostructure. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 167101.	0.2	2
18	Metal-embedded nitrogen-doped graphene for H2O molecule dissociation. Carbon, 2017, 115, 773-780.	5.4	50

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19	Elastic, electronic and optical properties of stable pentagonal ZnO 2. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 91, 82-87.	1.3	26
20	Enhanced thermoelectric properties of penta-graphene by strain effects process. Materials Research Express, 2017, 4, 105031.	0.8	12
21	Tuning the electronic and magnetic properties of penta-graphene using a hydrogen atom: a theoretical study. RSC Advances, 2017, 7, 40200-40207.	1.7	34
22	Adsorption of formaldehyde molecule on the pristine and transition metal doped graphene: First-principles study. Applied Surface Science, 2017, 396, 1020-1025.	3.1	72
23	Thermoelectric Properties of Ce₃Te₄ under High Pressure: First-Principles Calculation. Materials Transactions, 2017, 58, 1601-1605.	0.4	0
24	Molecular dynamics simulation of structural change at metal/semiconductor interface induced by nanoindenter. Chinese Physics B, 2016, 25, 114601.	0.7	1
25	Linear optical properties of defective KDP with oxygen vacancy: First-principles calculations. Chinese Physics B, 2015, 24, 077802.	0.7	12
26	A new class of â€œelectro-acid/baseâ€•induced reversible methyl ketone colour switches. Journal of Materials Chemistry C, 2013, 1, 5309.	2.7	40
27	Dynamic nano-pulling effect of the boron-functionalized graphene monovacancy for molecule dissociation. Journal Physics D: Applied Physics, 2013, 46, 385302.	1.3	10
28	Tuning of the periodicity of stable self-organized metallic templates. Chinese Physics B, 2011, 20, 020513.	0.7	0
29	Rare earth chalcogenide Ce3Te4 as high efficiency high temperature thermoelectric material. Applied Physics Letters, 2011, 98, .	1.5	18
30	Theoretical Investigations into Self-Organized Ordered Metallic Semi-Clusters Arrays on Metallic Substrate. Nanoscale Research Letters, 2010, 5, 1020-1026.	3.1	2
31	Ordered arrays of identicalNb4clusters on the GaN(0001) surface studied with first-principles calculations. Physical Review B, 2007, 75, .	1.1	9
32	First-principles calculations for the structural stabilities of orderedNb4clusters on theCu(111)surface. Physical Review B, 2006, 73, .	1.1	16
33	The geometric and electronic properties of the PbS, PbSe and PbTe (001) surfaces. Surface Science, 2004, 551, 91-98.	0.8	36
34	The calculation of the surface energy of high-index surfaces in metals at zero temperature. Surface Science, 2004, 551, 179-188.	0.8	44
35	The first principles investigation on Li or Sn codoped hexagonal tungsten bronzes as the near-infrared shielding material. Chinese Physics B, 0, , .	0.7	1