

Yu-Jun Zhao

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

189 papers	4,275 citations	36 h-index	58 g-index
195 ext. papers	4,977 ext. citations	4.3 avg, IF	5.58 L-index

#	Paper	IF	Citations
189	Theoretical study of magnetic phase transition in La ₂ Mn ₂ O ₇ . <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2022 , 432, 128010	2.3	
188	Theoretical Study of Oxygen-Vacancy Distribution in In ₂ O ₃ . <i>Journal of Physical Chemistry C</i> , 2021 , 125, 7077-7085	3.8	3
187	Mg adsorption on MgAl ₂ O ₄ surfaces and the effect of additive Ca: A combined experimental and theoretical study. <i>Journal of Alloys and Compounds</i> , 2021 , 861, 158564	5.7	1
186	Unconventional line defects engineering in two-dimensional boron monolayers. <i>Physical Review Materials</i> , 2021 , 5,	3.2	1
185	Theoretical study of tunable magnetism of two-dimensional MnS through strain, charge, and defect. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	2
184	Three-Dimensional Dirac Phonons with Inversion Symmetry. <i>Physical Review Letters</i> , 2021 , 126, 185301	7.4	8
183	Biased screening for multi-component materials with Structures of Alloy Generation And Recognition (SAGAR). <i>Computational Materials Science</i> , 2021 , 193, 110386	3.2	5
182	Gate-Controlled Magnetic Phase Transition in a van der Waals Magnet FeGeTe. <i>Nano Letters</i> , 2021 , 21, 5599-5605	11.5	8
181	First-principles study of aziridinium tin iodide perovskites for photovoltaics. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 982-990	7.1	3
180	All-boron planar ferromagnetic structures: from clusters to monolayers. <i>Nanoscale</i> , 2021 , 13, 9881-9887	7.7	1
179	Interface of Sn-doped AgAlTe ₂ and LiInTe ₂ : A theoretical model of tandem intermediate band absorber. <i>Applied Physics Letters</i> , 2021 , 118, 043901	3.4	1
178	In situ and tunable structuring of semiconductor-in-glass transparent composite. <i>IScience</i> , 2021 , 24, 101984	1.8	5
177	Theoretical investigation of the surface orientation impact on the hydrogen vacancy formation of MgH ₂ . <i>Surface Science</i> , 2021 , 710, 121850	1.8	0
176	Atom Classification Model for Total Energy Evaluation of Two-Dimensional Multicomponent Materials. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 4506-4511	2.8	7
175	Ideal type-III nodal-ring phonons. <i>Physical Review B</i> , 2020 , 101,	3.3	16
174	Theoretical study of active Ca element on grain refining of carbon-inoculated Mg-Al alloy. <i>Materials and Design</i> , 2020 , 192, 108664	8.1	2
173	Motif based high-throughput structure prediction of superconducting monolayer titanium boride. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 16236-16243	3.6	3

172	Energy landscape of Au: a global view of structure transformation. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4402-4406	3.6	1
171	Theoretical study of strain induced magnetic transition of single-layer CrTe ₃ . <i>Journal of Applied Physics</i> , 2020 , 127, 033903	2.5	6
170	Doping induced charge density wave in monolayer TiS ₂ and phonon-mediated superconductivity. <i>Journal of Applied Physics</i> , 2020 , 127, 044301	2.5	5
169	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 2798-2805	7.1	7
168	Quantum Dynamics Simulation of Doublet Excitation and Magnetic Field Effect in Neutral Radical Materials. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 1194-1198	6.4	1
167	Theoretical study of stability and optical absorption properties of ferroelectric materials ZnXO ₃ (X=Ge, Sn and Pb). <i>Physica B: Condensed Matter</i> , 2020 , 580, 411748	2.8	1
166	Synthesis and Catalytic Properties of Porous Metal Silica Materials Templated and Functionalized by Extended Coordination Cages. <i>Inorganic Chemistry</i> , 2020 , 59, 767-776	5.1	8
165	Gate-Tuned Interlayer Coupling in van der Waals Ferromagnet Fe ₃ GeTe ₂ Nanoflakes. <i>Physical Review Letters</i> , 2020 , 125, 047202	7.4	33
164	Unexpected bowing band evolution in an all-inorganic CsSn Pb Br perovskite.. <i>RSC Advances</i> , 2020 , 10, 26407-26413	3.7	3
163	Theoretical study of enhanced ferromagnetism and tunable magnetic anisotropy of monolayer CrI ₃ by surface adsorption. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020 , 384, 126754	2.3	7
162	Dirac fermions in the antiferromagnetic spintronics material CuMnAs. <i>Physical Review B</i> , 2020 , 102,	3.3	2
161	Rational Design Principles of the Quantum Anomalous Hall Effect in Superlattice-like Magnetic Topological Insulators. <i>Physical Review Letters</i> , 2019 , 123, 096401	7.4	46
160	Sn-C and Se-C Co-Bonding SnSe/Few-Layered Graphene Micro-Nano Structure: Route to a Densely Compacted and Durable Anode for Lithium/Sodium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 36685-36696	9.5	36
159	Hydrogen adsorption, dissociation, and diffusion on high-index Mg(101 $\bar{1}$ 0) and their comparisons with Mg(0001): A systematic first-principles study. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 4897-4906	6.7	8
158	Influence of Ca adsorption on the heterogeneous nucleation of Mg on Al ₄ C ₃ particles: First-principles calculation and experiment. <i>Applied Surface Science</i> , 2019 , 491, 187-194	6.7	9
157	Theoretical study of MH ₂ (M=Ti, V, Zr or Nb) structure phase diagram at high pressures. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 13592-13605	6.7	2
156	Transition metal substitution on Mg(101 $\bar{1}$ 0) and Mg(0001) surfaces for improved hydrogenation and dehydrogenation: A systematic first-principles study. <i>Applied Surface Science</i> , 2019 , 479, 626-633	6.7	2
155	Insights into the unusual semiconducting behavior in low-dimensional boron. <i>Nanoscale</i> , 2019 , 11, 7866-7874	7.4	2

- 154 Role of intrinsic defects on the persistent luminescence of pristine and Mn doped ZnGa₂O₄. *Journal of Applied Physics*, **2019**, 125, 095701 2.5 4
- 153 Understanding the Decomposition Mechanisms of LiNH₂, Mg(NH₂)₂, and NaNH₂: A Joint Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 18180-18186 3.8 6
- 152 Tunable ferromagnetic Weyl fermions from a hybrid nodal ring. *Npj Computational Materials*, **2019**, 5, 10.9 11
- 151 Theoretical investigations on stable structures of C₆₀-nNn (n=2-12): Symmetry, model interaction, and global optimization. *Carbon*, **2019**, 154, 140-149 10.4 3
- 150 Pressureless Crystallization of Glass for Transparent Nanoceramics. *Advanced Science*, **2019**, 6, 1901096 13.6 13
- 149 Antisymmetric magnetoresistance in van der Waals FeGeTe/graphite/FeGeTe trilayer heterostructures. *Science Advances*, **2019**, 5, eaaw0409 14.3 57
- 148 Coordination Geometry Engineering in a Doped Disordered Matrix for Tunable Optical Response. *Journal of Physical Chemistry C*, **2019**, 123, 29343-29352 3.8 8
- 147 Ideal half-filled intermediate band position in CuGaS₂ generated by Sb-related defect complex: a first-principles study. *Applied Physics Express*, **2019**, 12, 021002 2.4 2
- 146 Mg-X (X = Ni, Pd, Ti, Nb) interface and atomic mixture effect: a first-principles study. *Materials Research Express*, **2019**, 6, 016305 1.7 1
- 145 First-Principles Study of Aziridinium Lead Iodide Perovskite for Photovoltaics. *ChemPhysChem*, **2019**, 20, 602-607 3.2 2
- 144 First-principles study of ZnO/Mg heterogeneous nucleation interfaces. *Materials Research Express*, **2018**, 5, 036519 1.7 6
- 143 Theoretical investigations on diamondoids (CH_n, n = 10-41): Nomenclature, structural stabilities, and gap distributions. *Journal of Chemical Physics*, **2018**, 148, 014306 3.9 2
- 142 First-principles study on the stability and magnetoelectric properties of multiferroic materials XTiO₃ (X = Mn, Fe, Co, Ni). *International Journal of Modern Physics B*, **2018**, 32, 1850105 1.1 3
- 141 Theoretical study of YFe₂H (x = 0-1): A comparison between cubic and orthorhombic phases. *Journal of Magnetism and Magnetic Materials*, **2018**, 460, 61-68 2.8 10
- 140 Role of organic cations on hybrid halide perovskite CH₃NH₃PbI₃ surfaces. *Journal of Solid State Chemistry*, **2018**, 258, 488-494 3.3 9
- 139 Transition Metal Doped Smart Glass with Pressure and Temperature Sensitive Luminescence. *Advanced Optical Materials*, **2018**, 6, 1800881 8.1 29
- 138 An electron compensation mechanism for the polymorphism of boron monolayers. *Nanoscale*, **2018**, 10, 13410-13416 7.7 11
- 137 General rules of the sub-band gaps in group-IV (Si, Ge, and Sn)-doped I-III-VI₂-type chalcopyrite compounds for intermediate band solar cell: A first-principles study. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **2018**, 236-237, 147-152 3.1 12

136	Large-gap quantum anomalous Hall phase in hexagonal organometallic frameworks. <i>Physical Review B</i> , 2018 , 98,	3.3	11
135	Reverse Saturable Absorption Induced by Phonon-Assisted Anti-Stokes Processes. <i>Advanced Materials</i> , 2018 , 30, e1801638	24	39
134	The electronic properties of CH ₃ NH ₃ PbI ₃ perovskite surfaces tuned by inverted polarities of pyridine and ethylamine. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 6733-6738	7.1	3
133	Achieving the dehydriding reversibility and elevating the equilibrium pressure of YFe ₂ alloy by partial Y substitution with Zr. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 14541-14549	6.7	15
132	Group-IV (Si, Ge, and Sn)-doped AgAlTe ₂ for intermediate band solar cell from first-principles study. <i>Semiconductor Science and Technology</i> , 2017 , 32, 065007	1.8	11
131	The role of oxygen defects in a bismuth doped ScVO ₄ matrix: tuning luminescence by hydrogen treatment. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 314-321	7.1	12
130	Effects of organic cations on the defect physics of tin halide perovskites. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 15124-15129	13	135
129	Difficulty of long-standing n-type conductivity in equilibrium and non-equilibrium β -CuCl: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017 , 381, 2743-2747	2.7	3
128	Stable sandwich structures of two-dimensional iron borides FeB _x alloy: a first-principles calculation. <i>RSC Advances</i> , 2017 , 7, 30320-30326	3.7	4
127	Minimum Vertex-type Sequence Indexing for Clusters on Square Lattice. <i>Scientific Reports</i> , 2017 , 7, 392	4.9	3
126	High-Performance Color-Tunable Perovskite Light Emitting Devices through Structural Modulation from Bulk to Layered Film. <i>Advanced Materials</i> , 2017 , 29, 1603157	24	172
125	Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 29237-29243	3.6	24
124	Role of metal impurity in hydrogen diffusion from surface into bulk magnesium: A theoretical study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2017 , 381, 3696-3700	2.3	3
123	Geometrical eigen-subspace framework based molecular conformation representation for efficient structure recognition and comparison. <i>Journal of Chemical Physics</i> , 2017 , 146, 154108	3.9	13
122	An intrinsic representation of atomic structure: From clusters to periodic systems. <i>Journal of Chemical Physics</i> , 2017 , 147, 144106	3.9	8
121	Gap maximum of graphene nanoflakes: a first-principles study combined with the Monte Carlo tree search method. <i>RSC Advances</i> , 2017 , 7, 37881-37886	3.7	4
120	First-Principles Calculations of Quantum Efficiency for Point Defects in Semiconductors: The Example of Yellow Luminescence by GaN: CN+ON and GaN:CN. <i>Advanced Optical Materials</i> , 2017 , 5, 1700404	8.1	20
119	3D Foam Strutted Graphene Carbon Nitride with Highly Stable Optoelectronic Properties. <i>Advanced Functional Materials</i> , 2017 , 27, 1703711	15.6	64

118	Two-Dimensional Semiconducting Boron Monolayers. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17233-17236	16.4	34
117	Structural stabilities and electronic properties of Mg ₂₈ -nAl _n clusters: A first-principles study. <i>AIP Advances</i> , 2017 , 7, 095023	1.5	7
116	An extended cluster expansion for ground states of heterofullerenes. <i>Scientific Reports</i> , 2017 , 7, 16211	4.9	6
115	A Practical Criterion for Screening Stable Boron Nanostructures. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 11950-11955	3.8	12
114	Theoretical investigations of the interaction between transition-metal and benzoquinone: Metal dispersion and hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2016 , 41, 11275-11283	6.7	6
113	The structural evolution of hydrogenated silicon carbide nanocrystals: an approach from bond energy model, Wang-Landau method and first-principles studies. <i>Journal Physics D: Applied Physics</i> , 2016 , 49, 245305	3	1
112	Understanding the high p-type conductivity in Cu-excess CuAlS ₂ : A first-principles study. <i>Applied Physics Express</i> , 2016 , 9, 031202	2.4	5
111	The nucleation and growth of borophene on the Ag (111) surface. <i>Nano Research</i> , 2016 , 9, 2616-2622	10	66
110	High-coverage stable structures of 3d transition metal intercalated bilayer graphene. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14244-51	3.6	9
109	Complexity of H-bonding between polar molecules on Si(100)-2 × 1 and Ge(100)-2 × 1 surfaces. <i>Surface Science</i> , 2016 , 651, 187-194	1.8	5
108	Temperature effect on the structural stabilities and electronic properties of X ₂₂ H ₂₈ (X=C, Si and Ge) nanocrystals: A first-principles study. <i>AIP Advances</i> , 2016 , 6, 125112	1.5	
107	Competition between Pauli Exclusion and H-Bonding: H ₂ O and NH ₃ on Silicene. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 19151-19159	3.8	5
106	Understanding the stable boron clusters: A bond model and first-principles calculations based on high-throughput screening. <i>Journal of Chemical Physics</i> , 2015 , 142, 214307	3.9	22
105	Quasilattice-Conserved Optimization of the Atomic Structure of Decagonal Al-Co-Ni Quasicrystals. <i>Chinese Physics Letters</i> , 2015 , 32, 036102	1.8	0
104	Express penetration of hydrogen on Mg(10 13) along the close-packed-planes. <i>Scientific Reports</i> , 2015 , 5, 10776	4.9	81
103	First-principles study of Mg/Al ₂ MgC ₂ heterogeneous nucleation interfaces. <i>Applied Surface Science</i> , 2015 , 355, 1091-1097	6.7	37
102	Theoretical search for half-Heusler topological insulators. <i>Physical Review B</i> , 2015 , 91,	3.3	34
101	Controllable hydrogen adsorption and desorption by strain modulation on Ti decorated defective graphene. <i>International Journal of Hydrogen Energy</i> , 2015 , 40, 12063-12071	6.7	25

100	First-principles study of electronic and optical properties of BiTiO ₃ . <i>Wuli Xuebao/Acta Physica Sinica</i> , 2015 , 64, 147102	0.6	1
99	Order-disorder phase transitions in the two-dimensional semiconducting transition metal dichalcogenide alloys Mo(1-x)W(x)X ₂ (X = S, Se, and Te). <i>Scientific Reports</i> , 2014 , 4, 6691	4.9	45
98	H-Bond Interaction-Enhanced Dissociation of H ₂ O on Si(100)-2 \times 1. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 24603-24610	3.8	4
97	Symbiotic CeH _{2.73} /CeO ₂ catalyst: A novel hydrogen pump. <i>Nano Energy</i> , 2014 , 9, 80-87	17.1	115
96	Tuning p/n conductivity in wurtzite transition metal monoxide: Role of native defects in CoO and MnO. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014 , 378, 2635-2639	2.3	7
95	Theoretical studies of geometry asymmetry in tellurium nanostructures: intrinsic dipole, charge separation, and semiconductor-metal transition. <i>RSC Advances</i> , 2014 , 4, 44004-44010	3.7	2
94	Theoretical study of stability and electronic structure of the new type of ferroelectric materials XSnO ₃ (X = Mn, Zn, Fe, Mg). <i>International Journal of Modern Physics B</i> , 2014 , 28, 1450224	1.1	10
93	A systematic first-principles study of surface energies, surface relaxation and Friedel oscillation of magnesium surfaces. <i>Journal Physics D: Applied Physics</i> , 2014 , 47, 115305	3	29
92	The oxygen octahedral distortion induced magnetic enhancement in multiferroic Bi _{1-x} Yb _x Fe _{0.95} Co _{0.05} O ₃ powders. <i>Journal of Alloys and Compounds</i> , 2014 , 604, 327-330	5.7	18
91	First-principles prediction of a promising p-type transparent conductive material CsGeCl ₃ . <i>Applied Physics Express</i> , 2014 , 7, 041201	2.4	6
90	Structure, electronic and electrochemical properties of Li-rich metal phosphate by first-principles study. <i>Journal Physics D: Applied Physics</i> , 2014 , 47, 025301	3	2
89	Modeling and stabilities of Mg/MgH ₂ interfaces: A first-principles investigation. <i>AIP Advances</i> , 2014 , 4, 077101	1.5	11
88	First-principle prediction of robust half-metallic Te-based half-Heusler alloys. <i>Journal of Magnetism and Magnetic Materials</i> , 2014 , 350, 119-123	2.8	18
87	Gd ₃ B(W,Mo)O ₉ : Eu ³⁺ red phosphor: From structure design to photoluminescence behavior and near-UV white-LEDs performance. <i>Journal of Alloys and Compounds</i> , 2014 , 610, 402-408	5.7	39
86	Theoretical study of magnetic phase transitions of cubic SrMnO ₃ under physical and chemical pressures. <i>Computational Materials Science</i> , 2014 , 83, 394-397	3.2	7
85	Theoretical study of structural stabilities and magnetic properties of doped transition metals in MnTe vs ZnTe and CdTe: Reduced clustering trend and enhanced magnetic coupling. <i>Journal of Applied Physics</i> , 2013 , 114, 083905	2.5	2
84	First-principles study of the formation and migration of native defects in LiNH ₂ BH ₃ . <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 893-900	3.6	7
83	Structural stability of Cr-related defect complex in diamond for single photon sources: A first-principles study. <i>Journal of Applied Physics</i> , 2013 , 113, 103516	2.5	4

82	First-principles analysis of MoS ₂ /Ti ₂ C and MoS ₂ /Ti ₂ CY ₂ (Y=F and OH) all-2D semiconductor/metal contacts. <i>Physical Review B</i> , 2013 , 87,	3.3	133
81	The magnetoelectric properties of A- or B-site-doped PbVO ₃ films: A first-principles study. <i>Chinese Physics B</i> , 2013 , 22, 087703	1.2	1
80	Theoretical studies of the passivants' effect on the Si(x)Ge(1-x) nanowires: composition profiles, diameter, shape, and electronic properties. <i>Journal of Chemical Physics</i> , 2013 , 139, 154713	3.9	
79	THE STRUCTURE, MAGNETISM AND CONDUCTIVITY OF Li ₃ V ₂ (PO ₄) ₃ : A THEORETICAL AND EXPERIMENTAL STUDY. <i>Modern Physics Letters B</i> , 2013 , 27, 1350199	1.6	3
78	Theoretical study of structural stabilities of BiXO ₃ (X= Cr, Mn, Fe, Ni). <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013 , 62, 053102	0.6	1
77	Influences of strain on electronic structure and magnetic properties of CoFe ₂ O ₄ from first-principles study. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2013 , 62, 167502	0.6	2
76	First-principles study of the structural, magnetic, and electronic properties of LiMBO ₃ (M = Mn, Fe, Co). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 376, 179-184	2.3	15
75	Transition-metal dispersion on carbon-doped boron nitride nanostructures: Applications for high-capacity hydrogen storage. <i>Physical Review B</i> , 2012 , 86,	3.3	41
74	Inverse NiO _{1-x} /Cu Catalyst with High Activity toward Water-Gas Shift. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 16089-16092	3.8	16
73	First-principles study of ECuI for p-type transparent conducting materials. <i>Journal Physics D: Applied Physics</i> , 2012 , 45, 145102	3	29
72	First-Principles Study of Biaxial Strain Effect on Hydrogen Adsorbed Mg (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 14943-14949	3.8	21
71	Catalytic Reactivity of CuNi Alloys toward H ₂ O and CO Dissociation for an Efficient Water-Gas Shift: A DFT Study. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 745-752	3.8	59
70	Theoretical study of hydrogen dissociation and diffusion on Nb and Ni co-doped Mg(0001): A synergistic effect. <i>Surface Science</i> , 2012 , 606, L45-L49	1.8	21
69	First-principles prediction of a new class of photovoltaic materials: I-III-IV ₂ -V ₄ phosphides. <i>Journal of Applied Physics</i> , 2012 , 112, 053102	2.5	4
68	Stability of transition metals on Mg(0001) surfaces and their effects on hydrogen adsorption. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 309-317	6.7	43
67	Surface structure and phase transition of K adsorption on Au(111): by ab initio atomistic thermodynamics. <i>Journal of Chemical Physics</i> , 2012 , 136, 044510	3.9	6
66	Theoretical investigation of structural stability and electronic properties of hydrogenated silicon nanocrystals: Size, shape, and surface reconstruction. <i>Physical Review B</i> , 2012 , 86,	3.3	11
65	Tuning the polarization and magnetism in BiCoO ₃ by strain and oxygen vacancy effect: A first-principle study. <i>Journal of Applied Physics</i> , 2012 , 111, 013901	2.5	8

64	Ground states of group-IV nanostructures: Magic structures of diamond and silicon nanocrystals. <i>Physical Review B</i> , 2011 , 83,	3.3	13
63	Theoretical study of CO adsorption and oxidation on the gold-palladium bimetal clusters. <i>Computational and Theoretical Chemistry</i> , 2011 , 977, 62-68	2	41
62	AlH ₃ -mediated mechanism in hydriding/dehydriding of NaAlH ₄ . <i>International Journal of Hydrogen Energy</i> , 2011 , 36, 9767-9771	6.7	6
61	Theoretical study of the influence of Na on CO adsorption and dissociation on Pd(1 1 1): Long-range or short-range interactions between co-adsorbates?. <i>Chemical Physics Letters</i> , 2011 , 511, 33-38	2.5	10
60	Oxygen vacancy in LiTiPO ₅ and LiTi ₂ (PO ₄) ₃ : A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011 , 375, 934-938	2.3	21
59	Interaction between NO and Na, O, S, Cl on Au and Pd(111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 14466-75	3.6	7
58	Energetics and structure of single Ti defects and their influence on the decomposition of NaAlH ₄ . <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 552-62	3.6	9
57	Fe, Mn, and Cr doped BiCoO ₃ for magnetoelectric application: a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 326005	1.8	8
56	Pb codoping induced enhancement of ferromagnetism in Mn-doped In ₂ O ₃ : A first-principles study. <i>Physica B: Condensed Matter</i> , 2011 , 406, 1818-1821	2.8	10
55	Stability of BiAlO ₃ and its vacancy defects: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011 , 375, 633-637	2.3	10
54	Stable Antiferromagnetism of Orthorhombic BiCrO ₃ under Pressure: a Theoretical Study. <i>Advanced Materials Research</i> , 2011 , 298, 243-248	0.5	3
53	First-principles studies of Mn-doped LiCoPO ₄ . <i>Chinese Physics B</i> , 2011 , 20, 018201	1.2	6
52	Effect of biaxial strain on half-metallicity of transition metal alloyed zinc-blende ZnO and GaAs: a first-principles study. <i>Journal Physics D: Applied Physics</i> , 2011 , 44, 205002	3	5
51	First-principles study of Be doped CuAlS ₂ for p-type transparent conductive materials. <i>Journal of Applied Physics</i> , 2011 , 109, 113714	2.5	10
50	First-Principles Investigation of the Electronic Structure and Magnetic Properties for Co-Doped Fe ₃ O ₄ . <i>Materials Science Forum</i> , 2010 , 654-656, 1678-1681	0.4	
49	First-principles study of CuAlS ₂ for p-type transparent conductive materials. <i>Journal Physics D: Applied Physics</i> , 2010 , 43, 395405	3	14
48	Comparison of S Poisoning Effects on CO Adsorption on Pd, Au, and Bimetallic PdAu (111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 996-1003	3.8	33
47	Charge effect in S enhanced CO adsorption: A theoretical study of CO on Au, Ag, Cu, and Pd (111) surfaces coadsorbed with S, O, Cl, and Na. <i>Journal of Chemical Physics</i> , 2010 , 133, 094703	3.9	26

46	First-principles-based embedded atom method for PdAu nanoparticles. <i>Physical Review B</i> , 2009 , 80,	3.3	45
45	The origin of p-type conduction in (P, N) codoped ZnO. <i>Journal of Applied Physics</i> , 2009 , 106, 043707	2.5	35
44	Electronic structure and magnetic couplings in anatase TiO(2):V codoped with N, F, Cl. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 125502	1.8	9
43	Structural stability and magnetic properties of Co-doped or adsorbed polar-ZnO surface. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009 , 373, 391-395	2.3	12
42	The effect of oxygen vacancies on the structure and electrochemistry of LiTi ₂ (PO ₄) ₃ for lithium-ion batteries: A combined experimental and theoretical study. <i>Journal of Power Sources</i> , 2009 , 194, 1075-1080	8.9	93
41	Influence of Transition Metal Additives on the Hydriding/Dehydriding Critical Point of NaAlH ₄ . <i>Journal of Physical Chemistry C</i> , 2009 , 113, 9936-9943	3.8	19
40	Coverage-Dependent CO Adsorption Energy from First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 6088-6092	3.8	40
39	Magnetism and clustering in Cu doped ZnO. <i>Applied Physics Letters</i> , 2008 , 92, 182509	3.4	65
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