Yu-Jun Zhao

List of Publications by Year
in descending order

192	5,587	76326	98798
papers	citations	40 h-index	67 g-index

195	195	195	7232
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	n-type doping ofCuInSe2andCuGaSe2. Physical Review B, 2005, 72, .	3.2	429
2	Highâ€Performance Colorâ€Tunable Perovskite Light Emitting Devices through Structural Modulation from Bulk to Layered Film. Advanced Materials, 2017, 29, 1603157.	21.0	218
3	Effects of organic cations on the defect physics of tin halide perovskites. Journal of Materials Chemistry A, 2017, 5, 15124-15129.	10.3	213
4	First-principles analysis of MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>/Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>C and MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	3.2	166
5	Symbiotic CeH 2.73 /CeO 2 catalyst: A novel hydrogen pump. Nano Energy, 2014, 9, 80-87.	16.0	159
6	Room-Temperature Ferromagnetism in(Zn1â^'xMnx)GeP2Semiconductors. Physical Review Letters, 2002, 88, 257203.	7.8	151
7	Ruderman-Kittel-Kasuya-Yosidaâ€"like Ferromagnetism inMnxGe1â^'x. Physical Review Letters, 2003, 90, 047204.	7.8	148
8	Electronic structure of conducting polymers:â€ƒLimitations of oligomer extrapolation approximations and effects of heteroatoms. Physical Review B, 2003, 68, .	3.2	143
9	Antisymmetric magnetoresistance in van der Waals Fe ₃ GeTe ₂ /graphite/Fe ₃ GeTe ₂ trilayer heterostructures. Science Advances, 2019, 5, eaaw0409.	10.3	119
10	The effect of oxygen vacancies on the structure and electrochemistry of LiTi2(PO4)3 for lithium-ion batteries: A combined experimental and theoretical study. Journal of Power Sources, 2009, 194, 1075-1080.	7.8	107
11	Rational Design Principles of the Quantum Anomalous Hall Effect in Superlatticelike Magnetic Topological Insulators. Physical Review Letters, 2019, 123, 096401.	7.8	104
12	Structural, electronic, and magnetic properties of Î±- and Î²-MnAs: LDA and GGA investigations. Physical Review B, 2002, 65, .	3.2	92
13	Express penetration of hydrogen on Mg(10Íž13) along the close-packed-planes. Scientific Reports, 2015, 5, 10776.	3.3	89
14	3D Foam Strutted Graphene Carbon Nitride with Highly Stable Optoelectronic Properties. Advanced Functional Materials, 2017, 27, 1703711.	14.9	87
15	Gate-Tuned Interlayer Coupling in van der Waals Ferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow	7.8	87
16	Nanoflakes. Physical Review Letters, 2020, 125, 047202. The nucleation and growth of borophene on the Ag (111) surface. Nano Research, 2016, 9, 2616-2622.	10.4	86
17	Snâ€"C and Seâ€"C Co-Bonding SnSe/Few-Layered Graphene Microâ€"Nano Structure: Route to a Densely Compacted and Durable Anode for Lithium/Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 36685-36696.	8.0	83
18	Why can CuInSe2 be readily equilibrium-doped n-type but the wider-gap CuGaSe2 cannot?. Applied Physics Letters, 2004, 85, 5860-5862.	3.3	72

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19	Catalytic Reactivity of CuNi Alloys toward H₂O and CO Dissociation for an Efficient Waterâ€“Gas Shift: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 745-752.	3.1	71
20	Zinc-blende half-metallic ferromagnets are rarely stabilized by coherent epitaxy. Physical Review B, 2005, 71, .	3.2	68
21	Magnetism and clustering in Cu doped ZnO. Applied Physics Letters, 2008, 92, 182509.	3.3	67
22	Electronic and magnetic properties ofGa1âˆ’xMnxAs:Role of Mn defect bands. Physical Review B, 2001, 64, .	3.2	64
23	Three-Dimensional Dirac Phonons with Inversion Symmetry. Physical Review Letters, 2021, 126, 185301.	7.8	58
24	Two-Dimensional Semiconducting Boron Monolayers. Journal of the American Chemical Society, 2017, 139, 17233-17236.	13.7	57
25	Reverse Saturable Absorption Induced by Phononâ€Assisted Antiâ€Stokes Processes. Advanced Materials, 2018, 30, e1801638.	21.0	57
26	First-principles study of Mg/Al2MgC2 heterogeneous nucleation interfaces. Applied Surface Science, 2015, 355, 1091-1097.	6.1	55
27	Order-disorder phase transitions in the two-dimensional semiconducting transition metal dichalcogenide alloys Mo1âˆ’xWxX2 (X = S, Se and Te). Scientific Reports, 2014, 4, 6691.	3.3	54
28	Theoretical search for half-Heusler topological insulators. Physical Review B, 2015, 91, .	3.2	54
29	Magnetism of chalcopyrite semiconductors:Cd1âˆ’xMnxGeP2. Physical Review B, 2001, 63, .	3.2	53
30	First-principles-based embedded atom method for PdAu nanoparticles. Physical Review B, 2009, 80, .	3.2	53
31	Ideal type-III nodal-ring phonons. Physical Review B, 2020, 101, .	3.2	53
32	Electronic structure and ferromagnetism of Mn-substitutedCuAlS2,CuGaS2,CuInS2,CuGaSe2,andCuGaTe2. Physical Review B, 2004, 69, .	3.2	50
33	Coverage-Dependent CO Adsorption Energy from First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 6088-6092.	3.1	49
34	Stability of transition metals on Mg(0001) surfaces and their effects on hydrogen adsorption. International Journal of Hydrogen Energy, 2012, 37, 309-317.	7.1	48
35	Site preference for Mn substitution in spintronicCuMIIIX2VIchalcopyrite semiconductors. Physical Review B, 2004, 69, .	3.2	45
36	Transition-metal dispersion on carbon-doped boron nitride nanostructures: Applications for high-capacity hydrogen storage. Physical Review B, 2012, 86, .	3.2	45

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37	Gate-Controlled Magnetic Phase Transition in a van der Waals Magnet Fe₅GeTe₂. Nano Letters, 2021, 21, 5599-5605.	9.1	45
38	Theoretical study of CO adsorption and oxidation on the goldâ€“palladium bimetal clusters. Computational and Theoretical Chemistry, 2011, 977, 62-68.	2.5	44
39	Gd3B(W,Mo)O9: Eu3+ red phosphor: From structure design to photoluminescence behavior and near-UV white-LEDs performance. Journal of Alloys and Compounds, 2014, 610, 402-408.	5.5	44
40	Transition Metal Doped Smart Glass with Pressure and Temperature Sensitive Luminescence. Advanced Optical Materials, 2018, 6, 1800881.	7.3	43
41	Strong interface adhesion in Fe/TiC. Philosophical Magazine, 2005, 85, 3683-3697.	1.6	41
42	Possible impurity-induced ferromagnetism inIIâˆ’Geâˆ’V2chalcopyrite semiconductors. Physical Review B, 2002, 65, .	3.2	40
43	First-principles study of Î³-CuI for p-type transparent conducting materials. Journal Physics D: Applied Physics, 2012, 45, 145102.	2.8	40
44	The mechanism of Li, N dual-acceptor co-doped p-type ZnO. Applied Physics A: Materials Science and Processing, 2008, 91, 467-472.	2.3	39
45	A systematic first-principles study of surface energies, surface relaxation and Friedel oscillation of magnesium surfaces. Journal Physics D: Applied Physics, 2014, 47, 115305.	2.8	39
46	Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. Physical Chemistry Chemical Physics, 2017, 19, 29237-29243.	2.8	39
47	Mn-dopedCuGaS2chalcopyrites: Anab initiostudy of ferromagnetic semiconductors. Physical Review B, 2002, 66, .	3.2	38
48	Halogen n-type doping of chalcopyrite semiconductors. Applied Physics Letters, 2005, 86, 042109.	3.3	36
49	The origin of p-type conduction in (P, N) codoped ZnO. Journal of Applied Physics, 2009, 106, 043707.	2.5	36
50	Comparison of S Poisoning Effects on CO Adsorption on Pd, Au, and Bimetallic PdAu (111) Surfaces. Journal of Physical Chemistry C, 2010, 114, 996-1003.	3.1	35
51	Firstâ€Principles Calculations of Quantum Efficiency for Point Defects in Semiconductors: The Example of Yellow Luminance by GaN: C_N+O_N and GaN:C_N. Advanced Optical Materials, 2017, 5, 1700404.	7.3	33
52	First-principles prediction of a new class of ferromagnetic semiconductors. Journal of Magnetism and Magnetic Materials, 2002, 246, 145-150.	2.3	32
53	Comparison of predicted ferromagnetic tendencies of Mn substituting the Ga site in IIIâ€“Vâ€™s and in Iâ€“IIIâ€“VI2 chalcopyrite semiconductors. Applied Physics Letters, 2004, 84, 3753-3755.	3.3	32
54	Pushing p-type conductivity in ZnO by (Zr, N) codoping: A first-principles study. Solid State Communications, 2008, 147, 194-197.	1.9	32

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55	Controllable hydrogen adsorption and desorption by strain modulation on Ti decorated defective graphene. International Journal of Hydrogen Energy, 2015, 40, 12063-12071.	7.1	30
56	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. Journal of Chemical Physics, 2010, 133, 094703.	3.0	29
57	Pressureless Crystallization of Glass for Transparent Nanoceramics. Advanced Science, 2019, 6, 1901096.	11.2	29
58	Understanding the stable boron clusters: A bond model and first-principles calculations based on high-throughput screening. Journal of Chemical Physics, 2015, 142, 214307.	3.0	27
59	Oxygen vacancy in LiTiPO5 and LiTi2(PO4)3: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 934-938.	2.1	25
60	Advanced tetrahedrally-bonded magnetic semiconductors for spintronic applications. Journal of Physics and Chemistry of Solids, 2003, 64, 1453-1459.	4.0	24
61	First-Principles Study of Biaxial Strain Effect on Hydrogen Adsorbed Mg (0001) Surface. Journal of Physical Chemistry C, 2012, 116, 14943-14949.	3.1	24
62	First-principle prediction of robust half-metallic Te-based half-Heusler alloys. Journal of Magnetism and Magnetic Materials, 2014, 350, 119-123.	2.3	24
63	Influence of Transition Metal Additives on the Hydriding/Dehydriding Critical Point of NaAlH4. Journal of Physical Chemistry C, 2009, 113, 9936-9943.	3.1	23
64	The oxygen octahedral distortion induced magnetic enhancement in multiferroic Bi1â˜'xYbxFe0.95Co0.05O3 powders. Journal of Alloys and Compounds, 2014, 604, 327-330.	5.5	23
65	Practical rules for orbital-controlled ferromagnetism of 3d impurities in semiconductors. Journal of Applied Physics, 2005, 98, 113901.	2.5	21
66	Theoretical study of hydrogen dissociation and diffusion on Nb and Ni co-doped Mg(0001): A synergistic effect. Surface Science, 2012, 606, L45-L49.	1.9	21
67	Atomic displacements at aÎ£3(111)grain boundary inBaTiO3:A first-principles determination. Physical Review B, 2000, 63, .	3.2	20
68	Overlayer and superlattice studies of metal/ceramic interfaces: Fe/TiC. Journal of Applied Physics, 2003, 93, 6876-6878.	2.5	19
69	Inverse NiO_{1â€“x}/Cu Catalyst with High Activity toward Waterâ€“Gas Shift. Journal of Physical Chemistry C, 2012, 116, 16089-16092.	3.1	19
70	Achieving the dehydriding reversibility and elevating the equilibrium pressure of YFe2 alloy by partial Y substitution with Zr. International Journal of Hydrogen Energy, 2018, 43, 14541-14549.	7.1	19
71	An electron compensation mechanism for the polymorphism of boron monolayers. Nanoscale, 2018, 10, 13410-13416.	5.6	19
72	Influence of Ca adsorption on the heterogeneous nucleation of Î±-Mg on Al4C3 particles: First-principles calculation and experiment. Applied Surface Science, 2019, 491, 187-194.	6.1	19

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73	Theoretical Study of Oxygen-Vacancy Distribution in In₂O₃. Journal of Physical Chemistry C, 2021, 125, 7077-7085.	3.1	19
74	First-principles study of the structural, magnetic, and electronic properties of LiMBO3 (M=Mn, Fe, Co). Physics Letters, Section A: General, Atomic and Solid State Physics, 2012, 376, 179-184.	2.1	18
75	Large-gap quantum anomalous Hall phase in hexagonal organometallic frameworks. Physical Review B, 2018, 98, .	3.2	18
76	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.	3.5	17
77	Structural instability of epitaxial zinc-blende vanadium pnictides and chalcogenides for half-metallic ferromagnets. Journal of Applied Physics, 2008, 104, 053709.	2.5	16
78	First-principles study of CuAlS2for p-type transparent conductive materials. Journal Physics D: Applied Physics, 2010, 43, 395405.	2.8	16
79	Geometrical eigen-subspace framework based molecular conformation representation for efficient structure recognition and comparison. Journal of Chemical Physics, 2017, 146, 154108.	3.0	16
80	Synthesis and Catalytic Properties of Porous Metal Silica Materials Templated and Functionalized by Extended Coordination Cages. Inorganic Chemistry, 2020, 59, 767-776.	4.0	16
81	Theoretical study of enhanced ferromagnetism and tunable magnetic anisotropy of monolayer CrI3 by surface adsorption. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126754.	2.1	16
82	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. Journal of Materials Chemistry C, 2020, 8, 2798-2805.	5.5	16
83	The role of oxygen defects in a bismuth doped ScVO₄ matrix: tuning luminescence by hydrogen treatment. Journal of Materials Chemistry C, 2017, 5, 314-321.	5.5	15
84	Tunable ferromagnetic Weyl fermions from a hybrid nodal ring. Npj Computational Materials, 2019, 5, .	8.7	15
85	Biased screening for multi-component materials with Structures of Alloy Generation And Recognition (SAGAR). Computational Materials Science, 2021, 193, 110386.	3.0	15
86	Screened-exchange determination of the optical properties of large gap insulators: CaF2. Applied Physics Letters, 2004, 84, 3579-3581.	3.3	14
87	First-principles prediction of a promising p-type transparent conductive material CsGeCl₃. Applied Physics Express, 2014, 7, 041201.	2.4	14
88	Reconstruction of small Si cluster after ethylene adsorption: A full-potential linear-muffin-tin-orbital molecular-dynamics study. Journal of Chemical Physics, 1999, 110, 10738-10745.	3.0	13
89	Ground states of group-IV nanostructures: Magic structures of diamond and silicon nanocrystals. Physical Review B, 2011, 83, .	3.2	13
90	Modeling and stabilities of Mg/MgH2 interfaces: A first-principles investigation. AIP Advances, 2014, 4, .	1.3	13

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91	Theoretical study of YFe2H (xâ€¯=â€¯0â€“5): A comparison between cubic and orthorhombic phases. Journal of Magnetism and Magnetic Materials, 2018, 460, 61-68.	2.3	13
92	Atom Classification Model for Total Energy Evaluation of Two-Dimensional Multicomponent Materials. Journal of Physical Chemistry A, 2020, 124, 4506-4511.	2.5	13
93	A Practical Criterion for Screening Stable Boron Nanostructures. Journal of Physical Chemistry C, 2017, 121, 11950-11955.	3.1	13
94	Structural stability and magnetic properties of Co-doped or adsorbed polar-ZnO surface. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 391-395.	2.1	12
95	Fe, Mn, and Cr doped BiCoO₃for magnetoelectric application: a first-principles study. Journal of Physics Condensed Matter, 2011, 23, 326005.	1.8	12
96	Stability of BiAlO3 and its vacancy defects: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 633-637.	2.1	12
97	Tuning the polarization and magnetism in BiCoO3 by strain and oxygen vacancy effect: A first-principle study. Journal of Applied Physics, 2012, 111, 013901.	2.5	12
98	Theoretical study of stability and electronic structure of the new type of ferroelectric materials XSnO₃ (X = Mn, Zn, Fe, Mg). International Journal of Modern Physics B, 2014, 28, 1450224.	2.0	12
99	Group-IV (Si, Ge, and Sn)-doped AgAlTe₂for intermediate band solar cell from first-principles study. Semiconductor Science and Technology, 2017, 32, 065007.	2.0	12
100	Theoretical study of tunable magnetism of two-dimensional MnSe₂ through strain, charge, and defect. Journal of Physics Condensed Matter, 2021, 33, 215803.	1.8	12
101	A theoretical study of surfactant action in the layer-by-layer homoepitaxial growth of metals: the case of In on Cu(111). Physics Letters, Section A: General, Atomic and Solid State Physics, 1998, 239, 127-133.	2.1	11
102	Structural stability of(Ga,Mn)Asfrom first principles: Random alloys, ordered compounds, and superlattices. Physical Review B, 2006, 74, .	3.2	11
103	Theoretical study of the influence of Na on CO adsorption and dissociation on Pd(111): Long-range or short-range interactions between co-adsorbates?. Chemical Physics Letters, 2011, 511, 33-38.	2.6	11
104	First-principles studies of Mn-doped LiCoPO ₄. Chinese Physics B, 2011, 20, 018201.	1.4	11
105	Theoretical investigation of structural stability and electronic properties of hydrogenated silicon nanocrystals: Size, shape, and surface reconstruction. Physical Review B, 2012, 86, .	3.2	11
106	Hydrogen adsorption, dissociation, and diffusion on high-index Mg(10<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 162 Td (xmlns:m and their comparisons with Mg(0001): A systematic first-principles study. International Journal of Hydrogen Energy, 2019, 44, 4897-4906.	7.1	11
107	Theoretical study of strain induced magnetic transition of single-layer CrTe3. Journal of Applied Physics, 2020, 127, .	2.5	11
108	Surfactant-mediated layer-by-layer homoepitaxial growth ofCu/In/Cu(100)andAg/Sb/Ag(111)systems:â€ƒA theoretical study. Physical Review B, 1998, 57, 10054-10061.	3.2	10

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109	Interaction between NO and Na, O, S, Cl on Au and Pd(111) surfaces. Physical Chemistry Chemical Physics, 2011, 13, 14466.	2.8	10
110	Pâ€“n codoping induced enhancement of ferromagnetism in Mn-doped In2O3: A first-principles study. Physica B: Condensed Matter, 2011, 406, 1818-1821.	2.7	10
111	First-principles study of Be doped CuAlS2 for p-type transparent conductive materials. Journal of Applied Physics, 2011, 109, .	2.5	10
112	First-principles study of ZnO/Mg heterogeneous nucleation interfaces. Materials Research Express, 2018, 5, 036519.	1.6	10
113	Role of organic cations on hybrid halide perovskite CH3NH3PbI3 surfaces. Journal of Solid State Chemistry, 2018, 258, 488-494.	2.9	10
114	Coordination Geometry Engineering in a Doped Disordered Matrix for Tunable Optical Response. Journal of Physical Chemistry C, 2019, 123, 29343-29352.	3.1	10
115	Electronic structure and magnetic couplings in anatase TiO2:V codoped with N, F, Cl. Journal of Physics Condensed Matter, 2009, 21, 125502.	1.8	9
116	Energetics and structure of single Ti defects and their influence on the decomposition of NaAlH4. Physical Chemistry Chemical Physics, 2011, 13, 552-562.	2.8	9
117	Theoretical investigations of the interaction between transition-metal and benzoquinone: Metal dispersion and hydrogen storage. International Journal of Hydrogen Energy, 2016, 41, 11275-11283.	7.1	9
118	High-coverage stable structures of 3d transition metal intercalated bilayer graphene. Physical Chemistry Chemical Physics, 2016, 18, 14244-14251.	2.8	9
119	An intrinsic representation of atomic structure: From clusters to periodic systems. Journal of Chemical Physics, 2017, 147, 144106.	3.0	9
120	An extended cluster expansion for ground states of heterofullerenes. Scientific Reports, 2017, 7, 16211.	3.3	9
121	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.	3.1	9
122	Role of intrinsic defects on the persistent luminescence of pristine and Mn doped ZnGa2O4. Journal of Applied Physics, 2019, 125, .	2.5	9
123	Doping induced charge density wave in monolayer TiS2 and phonon-mediated superconductivity. Journal of Applied Physics, 2020, 127, 044301.	2.5	9
124	Acetylene adsorption on Cu(111) and stepped Cu(111): theoretical study. Journal of Physics Condensed Matter, 1995, 7, 6449-6457.	1.8	8
125	Accurate heat of formation for fully hydrided<b />LaNi5 via the all-electron full-potential linearized augmented plane wave approach. Journal of Applied Physics, 2007, 102, .	2.5	8
126	Theoretical study of magnetic phase transitions of cubic SrMnO3 under physical and chemical pressures. Computational Materials Science, 2014, 83, 394-397.	3.0	8

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127	Tuning<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mi>p</mml:mi><mml:mo stretchy="false">/</mml:mo><mml:mi>n</mml:mi></mml:math>conductivity in wurtzite transition metal monoxide: Role of native defects in CoO and MnO. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 2635-2639.	2.1	8
128	Firstâ€Principles Study of Aziridinium Lead Iodide Perovskite for Photovoltaics. ChemPhysChem, 2019, 20, 602-607.	2.1	8
129	Dirac fermions in the antiferromagnetic spintronics material CuMnAs. Physical Review B, 2020, 102, .	3.2	8
130	Motif based high-throughput structure prediction of superconducting monolayer titanium boride. Physical Chemistry Chemical Physics, 2020, 22, 16236-16243.	2.8	8
131	Magnetism and electronic structure of Fe chains and nano-wires. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 1648-1649.	2.3	7
132	AlH3-mediated mechanism in hydriding/dehydriding of NaAlH4. International Journal of Hydrogen Energy, 2011, 36, 9767-9771.	7.1	7
133	Surface structure and phase transition of K adsorption on Au(111): By ab initio atomistic thermodynamics. Journal of Chemical Physics, 2012, 136, 044510.	3.0	7
134	First-principles study of the formation and migration of native defects in LiNH₂BH₃. Physical Chemistry Chemical Physics, 2013, 15, 893-900.	2.8	7
135	Stable sandwich structures of two-dimensional iron borides FeB_xalloy: a first-principles calculation. RSC Advances, 2017, 7, 30320-30326.	3.6	7
136	Structural stabilities and electronic properties of Mg28-nAln clusters: A first-principles study. AIP Advances, 2017, 7, 095023.	1.3	7
137	First-principles study of aziridinium tin iodide perovskites for photovoltaics. Journal of Materials Chemistry C, 2021, 9, 982-990.	5.5	7
138	All-boron planar ferromagnetic structures: from clusters to monolayers. Nanoscale, 2021, 13, 9881-9887.	5.6	7
139	Unconventional line defects engineering in two-dimensional boron monolayers. Physical Review Materials, 2021, 5, .	2.4	7
140	Toward ferromagnetic semimetal ground state with multiple Weyl nodes in van der Waals crystal MnSb₄Te₇. New Journal of Physics, 2022, 24, 043033.	2.9	7
141	Ab initiomolecular dynamics study of adsorption and restoration: Si(100):Se. Journal of Physics Condensed Matter, 1998, 10, 7769-7776.	1.8	6
142	Structural stability of Cr-related defect complex in diamond for single photon sources: A first-principles study. Journal of Applied Physics, 2013, 113, .	2.5	6
143	Transition metal substitution on Mg(101Â¯3) and Mg(0001) surfaces for improved hydrogenation and dehydrogenation: A systematic first-principles study. Applied Surface Science, 2019, 479, 626-633.	6.1	6
144	Interface of Sn-doped AgAlTe2 and LiInTe2: A theoretical model of tandem intermediate band absorber. Applied Physics Letters, 2021, 118, .	3.3	6

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145	In situ and tunable structuring of semiconductor-in-glass transparent composite. IScience, 2021, 24, 101984.	4.1	6
146	Nanostructured Glass Composite for Selfâ€Calibrated Radiation Dose Rate Detection. Advanced Optical Materials, 0, , 2100751.	7.3	6
147	Effect of biaxial strain on half-metallicity of transition metal alloyed zinc-blende ZnO and GaAs: a first-principles study. Journal Physics D: Applied Physics, 2011, 44, 205002.	2.8	5
148	THE STRUCTURE, MAGNETISM AND CONDUCTIVITY OF Li3V2(PO4)3: A THEORETICAL AND EXPERIMENTAL STUDY. Modern Physics Letters B, 2013, 27, 1350199.	1.9	5
149	Competition between Pauli Exclusion and H-Bonding: H2O and NH3 on Silicene. Journal of Physical Chemistry C, 2016, 120, 19151-19159.	3.1	5
150	Understanding the high p-type conductivity in Cu-excess CuAlS₂: A first-principles study. Applied Physics Express, 2016, 9, 031202.	2.4	5
151	Complexity of H-bonding between polar molecules on Si(100)-2 Ã— 1 and Ge(100)-2 Ã— 1 surfaces. Surface Science, 2016, 651, 187-194.	1.9	5
152	Role of metal impurity in hydrogen diffusion from surface into bulk magnesium: A theoretical study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 3696-3700.	2.1	5
153	Gap maximum of graphene nanoflakes: a first-principles study combined with the Monte Carlo tree search method. RSC Advances, 2017, 7, 37881-37886.	3.6	5
154	Theoretical study of active Ca element on grain refining of carbon-inoculated Mg-Al alloy. Materials and Design, 2020, 192, 108664.	7.0	5
155	Theoretical investigation of the surface orientation impact on the hydrogen vacancy formation of MgH2. Surface Science, 2021, 710, 121850.	1.9	5
156	The adsorption and reaction pathway of dehydrogenated ethylene on Ni(111): a theoretical study. Journal of Physics Condensed Matter, 1997, 9, 9507-9515.	1.8	4
157	Stable Antiferromagnetism of Orthorhombic BiCrO₃ under Pressure: a Theoretical Study. Advanced Materials Research, 0, 298, 243-248.	0.3	4
158	First-principles prediction of a new class of photovoltaic materials: I-III-IV2-V4 phosphides. Journal of Applied Physics, 2012, 112, 053102.	2.5	4
159	H-Bond Interaction-Enhanced Dissociation of H₂O on Si(100)-2Ã—1. Journal of Physical Chemistry C, 2014, 118, 24603-24610.	3.1	4
160	Difficulty of long-standing n-type conductivity in equilibrium and non-equilibrium Î³ -CuCl: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 2743-2747.	2.1	4
161	Theoretical investigations on diamondoids (CnHm, n = 10â€“41): Nomenclature, structural stabilities, and gap distributions. Journal of Chemical Physics, 2018, 148, 014306.	3.0	4
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