Yu-Jun Zhao

List of Publications by Citations

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	n-type doping of CuInSe2 and CuGaSe2. *Physical Review B*, **2005**, 72,	3.3	384
188	High-Performance Color-Tunable Perovskite Light Emitting Devices through Structural Modulation from Bulk to Layered Film. *Advanced Materials*, **2017**, 29, 1603157	24	172
187	Room-temperature ferromagnetism in (Zn1-xMnx)GeP2 semiconductors. *Physical Review Letters*, **2002**, 88, 257203	7.4	137
186	Effects of organic cations on the defect physics of tin halide perovskites. *Journal of Materials Chemistry A*, **2017**, 5, 15124-15129	13	135
185	First-principles analysis of MoS2/Ti2C and MoS2/Ti2CY2 (Y=F and OH) all-2D semiconductor/metal contacts. *Physical Review B*, **2013**, 87,	3.3	133
184	Electronic structure of conducting polymers: Limitations of oligomer extrapolation approximations and effects of heteroatoms. *Physical Review B*, **2003**, 68,	3.3	133
183	Ruderman-Kittel-Kasuya-Yosida-like ferromagnetism in MnxGe1-x. *Physical Review Letters*, **2003**, 90, 047204	7.4	131
182	Symbiotic CeH 2.73 /CeO 2 catalyst: A novel hydrogen pump. *Nano Energy*, **2014**, 9, 80-87	17.1	115
181	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	8.9	93
180	Express penetration of hydrogen on Mg(10 13) along the close-packed-planes. *Scientific Reports*, **2015**, 5, 10776	4.9	81
179	Structural, electronic, and magnetic properties of □and □MnAs: LDA and GGA investigations. *Physical Review B*, **2002**, 65,	3.3	81
178	Why can CuInSe2 be readily equilibrium-doped n-type but the wider-gap CuGaSe2 cannot?. *Applied Physics Letters*, **2004**, 85, 5860-5862	3.4	67
177	The nucleation and growth of borophene on the Ag (111) surface. *Nano Research*, **2016**, 9, 2616-2622	10	66
176	Zinc-blende half-metallic ferromagnets are rarely stabilized by coherent epitaxy. *Physical Review B*, **2005**, 71,	3.3	66
175	Magnetism and clustering in Cu doped ZnO. *Applied Physics Letters*, **2008**, 92, 182509	3.4	65
174	3D Foam Strutted Graphene Carbon Nitride with Highly Stable Optoelectronic Properties. *Advanced Functional Materials*, **2017**, 27, 1703711	15.6	64
173	Electronic and magnetic properties of Ga1□MnxAs: Role of Mn defect bands. *Physical Review B*, **2001**, 64,	3.3	63

172	Catalytic Reactivity of CuNi Alloys toward H2O and CO Dissociation for an Efficient Water□as Shift: A DFT Study. *Journal of Physical Chemistry C*, **2012**, 116, 745-752	3.8	59
171	Antisymmetric magnetoresistance in van der Waals FeGeTe/graphite/FeGeTe trilayer heterostructures. *Science Advances*, **2019**, 5, eaaw0409	14.3	57
170	Magnetism of chalcopyrite semiconductors: Cd1□MnxGeP2. *Physical Review B*, **2001**, 63,	3.3	50
169	Rational Design Principles of the Quantum Anomalous Hall Effect in Superlatticelike Magnetic Topological Insulators. *Physical Review Letters*, **2019**, 123, 096401	7.4	46
168	Order-disorder phase transitions in the two-dimensional semiconducting transition metal dichalcogenide alloys Mo(1-x)W(x)X□(X = S, Se, and Te). *Scientific Reports*, **2014**, 4, 6691	4.9	45
167	First-principles-based embedded atom method for PdAu nanoparticles. *Physical Review B*, **2009**, 80,	3.3	45
166	Stability of transition metals on Mg(0001) surfaces and their effects on hydrogen adsorption. *International Journal of Hydrogen Energy*, **2012**, 37, 309-317	6.7	43
165	Electronic structure and ferromagnetism of Mn-substituted CuAlS2, CuGaS2, CuInS2, CuGaSe2, and CuGaTe2. *Physical Review B*, **2004**, 69,	3.3	43
164	Site preference for Mn substitution in spintronic CuMIIIX2VI chalcopyrite semiconductors. *Physical Review B*, **2004**, 69,	3.3	43
163	Transition-metal dispersion on carbon-doped boron nitride nanostructures: Applications for high-capacity hydrogen storage. *Physical Review B*, **2012**, 86,	3.3	41
162	Theoretical study of CO adsorption and oxidation on the gold□palladium bimetal clusters. *Computational and Theoretical Chemistry*, **2011**, 977, 62-68	2	41
161	Coverage-Dependent CO Adsorption Energy from First-Principles Calculations. *Journal of Physical Chemistry C*, **2009**, 113, 6088-6092	3.8	40
160	Possible impurity-induced ferromagnetism in II□eV2 chalcopyrite semiconductors. *Physical Review B*, **2002**, 65,	3.3	40
159	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	5.7	39
158	Reverse Saturable Absorption Induced by Phonon-Assisted Anti-Stokes Processes. *Advanced Materials*, **2018**, 30, e1801638	24	39
157	First-principles study of Mg/Al2MgC2 heterogeneous nucleation interfaces. *Applied Surface Science*, **2015**, 355, 1091-1097	6.7	37
156	The mechanism of Li, N dual-acceptor co-doped p-type ZnO. *Applied Physics A: Materials Science and Processing*, **2008**, 91, 467-472	2.6	37
155	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. *ACS Applied Materials & Interfaces*, **2019**, 11, 36685-36696	9.5	36

154	Strong interface adhesion in Fe/TiC. *Philosophical Magazine*, **2005**, 85, 3683-3697	1.6	36
153	Mn-doped CuGaS2 chalcopyrites: An ab initio study of ferromagnetic semiconductors. *Physical Review B*, **2002**, 66,	3.3	36
152	The origin of p-type conduction in (P, N) codoped ZnO. *Journal of Applied Physics*, **2009**, 106, 043707	2.5	35
151	Theoretical search for half-Heusler topological insulators. *Physical Review B*, **2015**, 91,	3.3	34
150	Two-Dimensional Semiconducting Boron Monolayers. *Journal of the American Chemical Society*, **2017**, 139, 17233-17236	16.4	34
149	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	3.8	33
148	Gate-Tuned Interlayer Coupling in van der Waals Ferromagnet Fe_{3}GeTe_{2} Nanoflakes. *Physical Review Letters*, **2020**, 125, 047202	7.4	33
147	Pushing p-type conductivity in ZnO by (Zr, N) codoping: A first-principles study. *Solid State Communications*, **2008**, 147, 194-197	1.6	30
146	Comparison of predicted ferromagnetic tendencies of Mn substituting the Ga site in III□V□ and in I□II□V□2 chalcopyrite semiconductors. *Applied Physics Letters*, **2004**, 84, 3753-3755	3.4	30
145	First-principles prediction of a new class of ferromagnetic semiconductors. *Journal of Magnetism and Magnetic Materials*, **2002**, 246, 145-150	2.8	30
144	Transition Metal Doped Smart Glass with Pressure and Temperature Sensitive Luminescence. *Advanced Optical Materials*, **2018**, 6, 1800881	8.1	29
143	A systematic first-principles study of surface energies, surface relaxation and Friedel oscillation of magnesium surfaces. *Journal Physics D: Applied Physics*, **2014**, 47, 115305	3	29
142	First-principles study of □CuI for p-type transparent conducting materials. *Journal Physics D: Applied Physics*, **2012**, 45, 145102	3	29
141	Halogen n-type doping of chalcopyrite semiconductors. *Applied Physics Letters*, **2005**, 86, 042109	3.4	29
140	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	3.9	26
139	Controllable hydrogen adsorption and desorption by strain modulation on Ti decorated defective graphene. *International Journal of Hydrogen Energy*, **2015**, 40, 12063-12071	6.7	25
138	Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. *Physical Chemistry Chemical Physics*, **2017**, 19, 29237-29243	3.6	24
137	Understanding the stable boron clusters: A bond model and first-principles calculations based on high-throughput screening. *Journal of Chemical Physics*, **2015**, 142, 214307	3.9	22

136	Advanced tetrahedrally-bonded magnetic semiconductors for spintronic applications. *Journal of Physics and Chemistry of Solids*, **2003**, 64, 1453-1459	3.9	22
135	First-Principles Study of Biaxial Strain Effect on Hydrogen Adsorbed Mg (0001) Surface. *Journal of Physical Chemistry C*, **2012**, 116, 14943-14949	3.8	21
134	Theoretical study of hydrogen dissociation and diffusion on Nb and Ni co-doped Mg(0001): A synergistic effect. *Surface Science*, **2012**, 606, L45-L49	1.8	21
133	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	2.3	21
132	First-Principles Calculations of Quantum Efficiency for Point Defects in Semiconductors: The Example of Yellow Luminance by GaN: CN+ON and GaN:CN. *Advanced Optical Materials*, **2017**, 5, 1700404	8.1	20
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130	Influence of Transition Metal Additives on the Hydriding/Dehydriding Critical Point of NaAlH4. *Journal of Physical Chemistry C*, **2009**, 113, 9936-9943	3.8	19
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127	Atomic displacements at a Σ(111) grain boundary in BaTiO3: A first-principles determination. *Physical Review B*, **2000**, 63,	3.3	18
126	Overlayer and superlattice studies of metal/ceramic interfaces: Fe/TiC. *Journal of Applied Physics*, **2003**, 93, 6876-6878	2.5	17
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120	First-principles study of CuAlS2for p-type transparent conductive materials. *Journal Physics D: Applied Physics*, **2010**, 43, 395405	3	14
119	Geometrical eigen-subspace framework based molecular conformation representation for efficient structure recognition and comparison. *Journal of Chemical Physics*, **2017**, 146, 154108	3.9	13

118	Pressureless Crystallization of Glass for Transparent Nanoceramics. *Advanced Science*, **2019**, 6, 1901096	13.6	13
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116	Screened-exchange determination of the optical properties of large gap insulators: CaF2. *Applied Physics Letters*, **2004**, 84, 3579-3581	3.4	13
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111	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
110	Group-IV (Si, Ge, and Sn)-doped AgAlTe2for intermediate band solar cell from first-principles study. *Semiconductor Science and Technology*, **2017**, 32, 065007	1.8	11
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108	Tunable ferromagnetic Weyl fermions from a hybrid nodal ring. *Npj Computational Materials*, **2019**, 5,	10.9	11
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92	Electronic structure and magnetic couplings in anatase TiO(2):V codoped with N, F, Cl. *Journal of Physics Condensed Matter*, **2009**, 21, 125502	1.8	9
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88	Fe, Mn, and Cr doped BiCoO□for magnetoelectric application: a first-principles study. *Journal of Physics Condensed Matter*, **2011**, 23, 326005	1.8	8
87	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	8
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83	Gate-Controlled Magnetic Phase Transition in a van der Waals Magnet FeGeTe. *Nano Letters*, **2021**, 21, 5599-5605	11.5	8

82	Coordination Geometry Engineering in a Doped Disordered Matrix for Tunable Optical Response. *Journal of Physical Chemistry C*, **2019**, 123, 29343-29352	3.8	8
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80	Realizing graphene-like Dirac cones in triangular boron sheets by chemical functionalization. *Journal of Materials Chemistry C*, **2020**, 8, 2798-2805	7.1	7
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69	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
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41	Stable Antiferromagnetism of Orthorhombic BiCrO3 under Pressure: a Theoretical Study. *Advanced Materials Research*, **2011**, 298, 243-248	0.5	3
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38	Theoretical Study of Oxygen-Vacancy Distribution in In2O3. *Journal of Physical Chemistry C*, **2021**, 125, 7077-7085	3.8	3
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36	The electronic properties of CH3NH3PbI3 perovskite surfaces tuned by inverted polarities of pyridine and ethylamine. *Journal of Materials Chemistry C*, **2018**, 6, 6733-6738	7.1	3
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