Hai Yan Xiao

List of Publications by Year in Descending Order

103 papers	2,019 citations	28 h-index	40 g-index
111 ext. papers	2,546 ext. citations	4.6 avg, IF	5.04 L-index

#	Paper	IF	Citations
103	Electronic structure regulation toward the improvement of the hydrogenation properties of TiZrHfMoNb high-entropy alloy. *Journal of Alloys and Compounds*, **2022**, 905, 164150	5.7	0
102	Electronic structure and anion engineering for perovskite oxysulfide BaTi(O,S)3. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **2022**, 40, 012801	2.9	1
101	The origin of anomalous hydrogen occupation in high entropy alloys. *Journal of Materials Chemistry A*, **2022**, 10, 7228-7237	13	1
100	High-Temperature Thermoelectric Monolayer Bi2TeSe2 with High Power Factor and Ultralow Thermal Conductivity. *ACS Applied Energy Materials*, **2022**, 5, 2564-2572	6.1	3
99	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. *Journal of Physical Chemistry C*, **2022**, 126, 4751-4761	3.8	
98	Accelerating CO2 reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. *Chemical Engineering Journal*, **2022**, 446, 137161	14.7	1
97	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. *ACS Applied Materials & Interfaces*, **2021**,	9.5	5
96	Engineering Schottky-to-Ohmic contact transition for 2D metal□emiconductor junctions. *Applied Physics Letters*, **2021**, 118, 091601	3.4	11
95	Superior Hydrogen Sorption Kinetics of Ti0.20Zr0.20Hf0.20Nb0.40 High-Entropy Alloy. *Metals*, **2021**, 11, 470	2.3	2
94	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. *Metals*, **2021**, 11, 553	2.3	3
93	Approaching Charge Separation Efficiency to Unity without Charge Recombination. *Physical Review Letters*, **2021**, 126, 176401	7.4	16
92	Preliminary assessment of high-entropy alloys for tritium storage. *Tungsten*, **2021**, 3, 119-130	4.6	
91	A first-principles study of hydrogen storage of high entropy alloy TiZrVMoNb. *International Journal of Hydrogen Energy*, **2021**, 46, 21050-21058	6.7	6
90	Defect formation and its effect on the thermodynamic properties of Pu2Zr2O7 pyrochlore: a first-principles study. *Journal of the American Ceramic Society*, **2021**, 104, 2301-2312	3.8	0
89	The thermal and electrical transport properties of layered LaCuOSe under high pressure. *Journal of Alloys and Compounds*, **2021**, 861, 157984	5.7	5
88	A comparative study of the structural and optical properties of Si-doped GaAs under different ion irradiation. *Optical Materials*, **2021**, 111, 110611	3.3	6
87	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. *Inorganic Chemistry*, **2021**, 60, 1388-1397	5.1	6

86	Effect of Copper Doping on Electronic Structure and Optical Absorption of CdSe Quantum Dots. *Nanomaterials*, **2021**, 11,	5.4	1
85	The effect of hydrogen on the mechanical properties of high entropy alloy TiZrHfMoNb: First-principles investigation. *Journal of Alloys and Compounds*, **2021**, 879, 160482	5.7	7
84	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. *Npj Computational Materials*, **2021**, 7,	10.9	14
83	Electronic Structure, Optical Properties, and Photoelectrochemical Activity of Sn-Doped Fe2O3 Thin Films. *Journal of Physical Chemistry C*, **2020**, 124, 12548-12558	3.8	26
82	Effects of stacking periodicity on the electronic and optical properties of GaAs/AlAs superlattice: a first-principles study. *Scientific Reports*, **2020**, 10, 4862	4.9	3
81	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. *Inorganic Chemistry*, **2020**, 59, 9774-9782	5.1	16
80	Effects of temperature and energy on the radiation response of GaAs/AlAs and GaAs/AlGaAs superlattices. *Radiation Physics and Chemistry*, **2020**, 174, 108983	2.5	0
79	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. *Nanomaterials*, **2020**, 10,	5.4	1
78	Layered LaCuOSe: A Promising Anisotropic Thermoelectric Material. *Physical Review Applied*, **2020**, 13,	4.3	26
77	Compositional dependence of hydrogenation performance of Ti-Zr-Hf-Mo-Nb high-entropy alloys for hydrogen/tritium storage. *Journal of Materials Science and Technology*, **2020**, 55, 116-125	9.1	27
76	An abnormal incorporation behavior of Th in Gd2Zr2O7: A first-principles study. *Journal of the American Ceramic Society*, **2020**, 103, 1846-1853	3.8	0
75	MoO3 induces p-type surface conductivity by surface transfer doping in diamond. *Applied Surface Science*, **2020**, 509, 144890	6.7	18
74	A DFT+U study on the thermodynamic properties of defective Gd2Zr2O7 pyrochlore. *Journal of Nuclear Materials*, **2020**, 542, 152425	3.3	3
73	An AIMD+U simulation of low-energy displacement events in UO2. *Journal of Nuclear Materials*, **2020**, 540, 152379	3.3	0
72	Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 22758-22767	3.6	8
71	Electronic and nanostructure engineering of bifunctional MoS towards exceptional visible-light photocatalytic CO reduction and pollutant degradation. *Journal of Hazardous Materials*, **2020**, 381, 120972	12.8	52
70	High-electron-affinity oxide V2O5 enhances surface transfer doping on hydrogen-terminated diamond. *Diamond and Related Materials*, **2020**, 108, 107865	3.5	6
69	Electronic structure and p-type conduction mechanism of spinel cobaltite oxide thin films. *Physical Review B*, **2019**, 100,	3.3	32

68	A DFT study of the surface charge transfer doping of diamond by chromium trioxide. *Applied Surface Science*, **2019**, 496, 143604	6.7	11
67	Ab initio molecular dynamics simulation of the radiation damage effects of GaAs/AlGaAs superlattice. *Journal of Nuclear Materials*, **2019**, 516, 228-237	3.3	3
66	Optimizing the thermoelectric transport properties of BiOSe monolayer via biaxial strain. *Physical Chemistry Chemical Physics*, **2019**, 21, 15097-15105	3.6	27
65	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. *Nanomaterials*, **2019**, 9,	5.4	35
64	Elucidating the electronic structure of CuWO4 thin films for enhanced photoelectrochemical water splitting. *Journal of Materials Chemistry A*, **2019**, 7, 11895-11907	13	36
63	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd□r□□ *Nanomaterials*, **2019**, 9,	5.4	1
62	Improved thermoelectric performance of bilayer Bi2O2Se by the band convergence approach. *Journal of Materials Chemistry C*, **2019**, 7, 11029-11039	7.1	25
61	Effects of Ag doping on the electronic and optical properties of CdSe quantum dots. *Physical Chemistry Chemical Physics*, **2019**, 21, 16108-16119	3.6	31
60	High-Dose Electron Radiation and Unexpected Room-Temperature Self-Healing of Epitaxial SiC Schottky Barrier Diodes. *Nanomaterials*, **2019**, 9,	5.4	6
59	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. *Nanomaterials*, **2019**, 9,	5.4	39
58	A comparative study of low energy radiation response of AlAs, GaAs and GaAs/AlAs superlattice and the damage effects on their electronic structures. *Scientific Reports*, **2018**, 8, 2012	4.9	15
57	Orbital controlled band gap engineering of tetragonal BiFeO3 for optoelectronic applications. *Journal of Materials Chemistry C*, **2018**, 6, 1239-1247	7.1	49
56	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. *Nanoscale Research Letters*, **2018**, 13, 133	5	7
55	Effects of Nd doping on the mechanical properties and electronic structures of Gd2Zr2O7: a first-principles-based study. *Journal of Materials Science*, **2018**, 53, 16423-16438	4.3	16
54	First-Principles Study of Point Defects in GaAs/AlAs Superlattice: the Phase Stability and the Effects on the Band Structure and Carrier Mobility. *Nanoscale Research Letters*, **2018**, 13, 301	5	13
53	A comparative study of the mechanical and thermal properties of defective ZrC, TiC and SiC. *Scientific Reports*, **2017**, 7, 9344	4.9	19
52	Impact of isovalent and aliovalent substitution on the mechanical and thermal properties of GdZrO. *Scientific Reports*, **2017**, 7, 6399	4.9	14
51	Ab initio molecular dynamics simulation of low energy radiation responses of □AlO. *Scientific Reports*, **2017**, 7, 3621	4.9	8

50	Theoretical prediction of long-range ferromagnetism in transition-metal atom-doped d dichalcogenide single layers SnS and ZrS. *Physical Chemistry Chemical Physics*, **2016**, 18, 25151-25160	3.6	14
49	Atomistic Conversion Reaction Mechanism of WO3 in Secondary Ion Batteries of Li, Na, and Ca. *Angewandte Chemie*, **2016**, 128, 6352-6355	3.6	13
48	Engineering the electronic and magnetic properties of d(0) 2D dichalcogenide materials through vacancy doping and lattice strains. *Physical Chemistry Chemical Physics*, **2016**, 18, 7163-8	3.6	12
47	Atomistic Conversion Reaction Mechanism of WO3 in Secondary Ion Batteries of Li, Na, and Ca. *Angewandte Chemie - International Edition*, **2016**, 55, 6244-7	16.4	70
46	Ab initio molecular dynamics simulation of the effects of stacking faults on the radiation response of 3C-SiC. *Scientific Reports*, **2016**, 6, 20669	4.9	17
45	Structural, electronic and magnetic properties of metal□organic-framework perovskites [AmH][Mn(HCOO)3]: a first-principles study. *RSC Advances*, **2016**, 6, 48779-48787	3.7	10
44	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO□/SrTiO□ Heterostructures. *Nano Letters*, **2015**, 15, 4677-84	11.5	58
43	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. *Journal of Materials Chemistry C*, **2015**, 3, 3128-3134	7.1	6
42	Functionalization of a GaSe monolayer by vacancy and chemical element doping. *Physical Chemistry Chemical Physics*, **2015**, 17, 10737-48	3.6	30
41	Electronic excitation induced amorphization in titanate pyrochlores: an ab initio molecular dynamics study. *Scientific Reports*, **2015**, 5, 8265	4.9	15
40	Effects of surface defects on two-dimensional electron gas at NdAlO3/SrTiO3 interface. *Scientific Reports*, **2014**, 4, 5477	4.9	12
39	Nonlinear luminescence response of CaF2:Eu and YAlO3:Ce to single-ion excitation. *Journal of Applied Physics*, **2014**, 115, 033108	2.5	5
38	Effects of boron-nitride substrates on Stone-Wales defect formation in graphene: An ab initio molecular dynamics study. *Applied Physics Letters*, **2014**, 104, 203106	3.4	5
37	Coexistence of epitaxial lattice rotation and twinning tilt induced by surface symmetry mismatch. *Applied Physics Letters*, **2014**, 104, 221602	3.4	7
36	Structure and properties of rare earth silicates with the apatite structure at high pressure. *Physics and Chemistry of Minerals*, **2013**, 40, 817-825	1.6	7
35	Ab initio molecular dynamics simulations of ion□solid interactions in Gd2Zr2O7 and Gd2Ti2O7. *Journal of Materials Chemistry C*, **2013**, 1, 1665	7.1	31
34	The impact of crystal symmetry on the electronic structure and functional properties of complex lanthanum chromium oxides. *Journal of Materials Chemistry C*, **2013**, 1, 4527	7.1	37
33	Ab initio molecular dynamics simulations of threshold displacement energies in SrTiO3. *Journal of Physics Condensed Matter*, **2013**, 25, 485003	1.8	13

32	Nature of the band gap and origin of the electro-/photo-activity of Co3O4. *Journal of Materials Chemistry C*, **2013**, 1, 4628	7.1	127
31	Electronic Structure Calculations of A2Ti2O7(A = Dy, Ho, and Y). *Advances in Condensed Matter Physics*, **2013**, 2013, 1-8	1	4
30	Impact of point defects on electronic structure in Y2Ti2O7. *RSC Advances*, **2012**, 2, 7235	3.7	11
29	Enhanced electronic conductivity by controlled self-doping in pyrochlores. *Physical Chemistry Chemical Physics*, **2012**, 14, 6556-60	3.6	9
28	Ab initio molecular dynamics simulations of low-energy recoil events in ThO2, CeO2, and ZrO2. *Physical Review B*, **2012**, 86,	3.3	52
27	Structural and electronic properties of 0.5 ML sulfur adsorbed on the GaP(001) surface. *Journal of Materials Science*, **2011**, 46, 1635-1639	4.3	
26	Ab initio molecular dynamics simulation of pressure-induced phase transformation in BeO. *Journal of Materials Science*, **2011**, 46, 6408-6415	4.3	4
25	Pressure induced structural transformation in Gd□Ti□O□ and Gd□Zr□O□. *Journal of Physics Condensed Matter*, **2011**, 23, 035501	1.8	19
24	Oxygen vacancy formation and migration in Ce(x)Th(1-x)O2 solid solution. *Journal of Physical Chemistry B*, **2011**, 115, 6524-33	3.4	42
23	Functionalized graphene nanoroads for quantum well device. *Applied Physics Letters*, **2011**, 98, 093108	3.4	10
22	Threshold displacement energies and defect formation energies in Y2Ti2O7. *Journal of Physics Condensed Matter*, **2010**, 22, 415801	1.8	44
21	Zirconate pyrochlores under high pressure. *Physical Chemistry Chemical Physics*, **2010**, 12, 12472-7	3.6	39
20	Defect-enhanced charge transfer by ion-solid interactions in SiC using large-scale ab initio molecular dynamics simulations. *Physical Review Letters*, **2009**, 103, 027405	7.4	66
19	Threshold displacement energy in GaN: Ab initio molecular dynamics study. *Journal of Applied Physics*, **2009**, 105, 123527	2.5	70
18	ADSORPTION OF Li ON Mo(110) SURFACE: A FIRST-PRINCIPLES STUDY. *Surface Review and Letters*, **2009**, 16, 589-597	1.1	3
17	Ab initio molecular dynamics simulation of a pressure induced zinc blende to rocksalt phase transition in SiC. *Journal of Physics Condensed Matter*, **2009**, 21, 245801	1.8	8
16	Electronic and magnetic properties of graphene absorbed with S atom: A first-principles study. *Journal of Applied Physics*, **2009**, 105, 104311	2.5	28
15	Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. *Journal of Applied Physics*, **2009**, 105, 014309	2.5	86

14	First-principles calculation of structural and energetic properties for A2Ti2O7 (A = Lu, Er, Y, Gd, Sm, Nd, La). *Journal of Materials Research*, **2009**, 24, 1335-1341	2.5	33
13	Adsorption-induced magnetic properties and metallic behavior of graphene. *Applied Physics Letters*, **2009**, 95, 123119	3.4	57
12	Ab initio investigation of phase stability of Y2Ti2O7 and Y2Zr2O7 under high pressure. *Physical Review B*, **2009**, 80,	3.3	44
11	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. *Applied Physics Letters*, **2008**, 92, 183116	3.4	28
10	Ab initio calculations of structural and energetic properties of defects in gallium nitride. *Journal of Applied Physics*, **2008**, 103, 123529	2.5	13
9	First-principles study of energetic and electronic properties of A2Ti2O7 (A=Sm, Gd, Er) pyrochlore. *Journal of Applied Physics*, **2008**, 104, 073503	2.5	22
8	Structural phase transitions in high-pressure wurtzite to rocksalt phase in GaN and SiC. *Applied Physics Letters*, **2008**, 92, 241909	3.4	17
7	First-principles calculation of defect formation energies and electronic properties in stannate pyrochlores. *Journal of Applied Physics*, **2008**, 104, 093702	2.5	20
6	Effect of S adsorption on magnetic Co(0001) surface: a DFT study. *European Physical Journal B*, **2008**, 61, 319-324	1.2	3
5	Theoretical investigation of structural, energetic and electronic properties of titanate pyrochlores. *Journal of Physics Condensed Matter*, **2007**, 19, 346203	1.8	37
4	Atomistic simulation of helium-defect interaction in alpha-iron. *Applied Physics Letters*, **2006**, 88, 091915	3.4	41
3	First-principles study of the adsorption of cesium on Si(001)(2 x 1) surface. *Journal of Chemical Physics*, **2005**, 122, 174704	3.9	28
2	A DFT investigation of the adsorption of methyl on Rh(111). *Surface Science*, **2004**, 558, 15-22	1.8	20
1	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au6 Clusters. *ACS Applied Energy Materials*,	6.1	7