Hai Yan Xiao

List of Publications by Year
in descending order

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111 papers	3,090 citations	136740 32 h-index	189595 50 g-index
111 all docs	111 docs citations	111 times ranked	3826 citing authors

#	Article	IF	Citations
1	Nature of the band gap and origin of the electro-/photo-activity of Co3O4. Journal of Materials Chemistry C, 2013, 1, 4628.	2.7	176
2	Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. Journal of Applied Physics, 2009, 105, .	1.1	96
3	Electronic and nanostructure engineering of bifunctional MoS2 towards exceptional visible-light photocatalytic CO2 reduction and pollutant degradation. Journal of Hazardous Materials, 2020, 381, 120972.	6.5	90
4	Atomistic Conversion Reaction Mechanism of WO₃ in Secondary Ion Batteries of Li, Na, and Ca. Angewandte Chemie - International Edition, 2016, 55, 6244-6247.	7.2	86
5	Orbital controlled band gap engineering of tetragonal BiFeO₃ for optoelectronic applications. Journal of Materials Chemistry C, 2018, 6, 1239-1247.	2.7	80
6	Layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>La</mml:mi><mml:mi>Cu</mml:mi><mml:mi mathvariant="normal">O</mml:mi><mml:mi>Se</mml:mi></mml:mrow></mml:math> : A Promising Anisotropic Thermoelectric Material. Physical Review Applied, 2020, 13, .	1.5	80
7	Threshold displacement energy in GaN: Ab initio molecular dynamics study. Journal of Applied Physics, 2009, 105, .	1.1	79
8	Optimizing the thermoelectric transport properties of Bi₂O₂Se monolayer via biaxial strain. Physical Chemistry Chemical Physics, 2019, 21, 15097-15105.	1.3	76
9	Defect-Enhanced Charge Transfer by Ion-Solid Interactions in SiC using Large-ScaleAbÂInitioMolecular Dynamics Simulations. Physical Review Letters, 2009, 103, 027405.	2.9	74
10	Dimensionality Controlled Octahedral Symmetry-Mismatch and Functionalities in Epitaxial LaCoO₃/SrTiO₃ Heterostructures. Nano Letters, 2015, 15, 4677-4684.	4.5	71
11	Elucidating the electronic structure of CuWO₄ thin films for enhanced photoelectrochemical water splitting. Journal of Materials Chemistry A, 2019, 7, 11895-11907.	5.2	67
12	A Novel TiZrHfMoNb High-Entropy Alloy for Solar Thermal Energy Storage. Nanomaterials, 2019, 9, 248.	1.9	66
13	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.	5.6	66
14	Band degeneracy enhanced thermoelectric performance in layered oxyselenides by first-principles calculations. Npj Computational Materials, 2021, 7, .	3.5	62
15	Adsorption-induced magnetic properties and metallic behavior of graphene. Applied Physics Letters, 2009, 95, 123119.	1.5	60
16	Ab initiomolecular dynamics simulations of low-energy recoil events in ThO<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>, CeO<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>, and ZrO<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>,	1.1	60
17	A DFT Study of Hydrogen Storage in High-Entropy Alloy TiZrHfScMo. Nanomaterials, 2019, 9, 461.	1.9	60
18	Electronic Structure, Optical Properties, and Photoelectrochemical Activity of Sn-Doped Fe₂O₃ Thin Films. Journal of Physical Chemistry C, 2020, 124, 12548-12558.	1.5	56

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19	Electronic structure and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math>-type conduction mechanism of spinel cobaltite oxide thin films. Physical Review B, 2019, 100, .	1.1	54
20	Improved thermoelectric performance of bilayer Bi₂O₂Se by the band convergence approach. Journal of Materials Chemistry C, 2019, 7, 11029-11039.	2.7	53
21	Threshold displacement energies and defect formation energies in Y₂Ti₂O₇. Journal of Physics Condensed Matter, 2010, 22, 415801.	0.7	50
22	Ab initioinvestigation of phase stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Y</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Y</mml:mtext><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2009, 80, .	1.1	48
23	Oxygen Vacancy Formation and Migration in Ce_xTh_{1â€“x}O₂ Solid Solution. Journal of Physical Chemistry B, 2011, 115, 6524-6533.	1.2	46
24	Atomistic simulation of helium-defect interaction in alpha-iron. Applied Physics Letters, 2006, 88, 091915.	1.5	44
25	Zirconate pyrochlores under high pressure. Physical Chemistry Chemical Physics, 2010, 12, 12472.	1.3	43
26	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.	2.7	42
27	Theoretical investigation of structural, energetic and electronic properties of titanate pyrochlores. Journal of Physics Condensed Matter, 2007, 19, 346203.	0.7	41
28	Ab initio molecular dynamics simulations of ionâ€“solid interactions in Gd2Zr2O7 and Gd2Ti2O7. Journal of Materials Chemistry C, 2013, 1, 1665.	2.7	40
29	Functionalization of a GaSe monolayer by vacancy and chemical element doping. Physical Chemistry Chemical Physics, 2015, 17, 10737-10748.	1.3	40
30	Effects of Ag doping on the electronic and optical properties of CdSe quantum dots. Physical Chemistry Chemical Physics, 2019, 21, 16108-16119.	1.3	38
31	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.	1.2	35
32	Approaching Charge Separation Efficiency to Unity without Charge Recombination. Physical Review Letters, 2021, 126, 176401.	2.9	35
33	High-Temperature Thermoelectric Monolayer Bi₂TeSe₂ with High Power Factor and Ultralow Thermal Conductivity. ACS Applied Energy Materials, 2022, 5, 2564-2572.	2.5	35
34	A comparative study of the mechanical and thermal properties of defective ZrC, TiC and SiC. Scientific Reports, 2017, 7, 9344.	1.6	34
35	Accelerating CO2 reduction on novel double perovskite oxide with sulfur, carbon incorporation: Synergistic electronic and chemical engineering. Chemical Engineering Journal, 2022, 446, 137161.	6.6	34
36	Boosting Thermoelectric Performance of 2D Transition-Metal Dichalcogenides by Complex Cluster Substitution: The Role of Octahedral Au₆ Clusters. ACS Applied Energy Materials, 2021, 4, 12163-12176.	2.5	33

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37	Electronic and magnetic properties of graphene absorbed with S atom: A first-principles study. Journal of Applied Physics, 2009, 105, .	1.1	32
38	A Density Functional Theory Study of the Hydrogen Absorption in High Entropy Alloy TiZrHfMoNb. Inorganic Chemistry, 2020, 59, 9774-9782.	1.9	31
39	MoO3 induces p-type surface conductivity by surface transfer doping in diamond. Applied Surface Science, 2020, 509, 144890.	3.1	30
40	Promoting the Oxygen Evolution Activity of Perovskite Nickelates through Phase Engineering. ACS Applied Materials & Interfaces, 2021, 13, 58566-58575.	4.0	30
41	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.	3.1	29
42	First-principles study of the adsorption of cesium on Si(001)(2Ã—1) surface. Journal of Chemical Physics, 2005, 122, 174704.	1.2	28
43	Tuning the band structures of single walled silicon carbide nanotubes with uniaxial strain: A first principles study. Applied Physics Letters, 2008, 92, 183116.	1.5	28
44	A first-principles study of hydrogen storage of high entropy alloy TiZrVMoNb. International Journal of Hydrogen Energy, 2021, 46, 21050-21058.	3.8	28
45	A DFT study of the surface charge transfer doping of diamond by chromium trioxide. Applied Surface Science, 2019, 496, 143604.	3.1	27
46	First-principles study of energetic and electronic properties of A2Ti2O7 (A=Sm, Gd, Er) pyrochlore. Journal of Applied Physics, 2008, 104, .	1.1	24
47	First-principles calculation of defect formation energies and electronic properties in stannate pyrochlores. Journal of Applied Physics, 2008, 104, .	1.1	23
48	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.	1.6	22
49	Engineering Schottky-to-Ohmic contact transition for 2D metalâ€“semiconductor junctions. Applied Physics Letters, 2021, 118, .	1.5	22
50	Ab initio molecular dynamics simulation of the effects of stacking faults on the radiation response of 3C-SiC. Scientific Reports, 2016, 6, 20669.	1.6	21
51	Atomistic Conversion Reaction Mechanism of WO₃ in Secondary Ion Batteries of Li, Na, and Ca. Angewandte Chemie, 2016, 128, 6352-6355.	1.6	21
52	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.	1.7	21
53	A DFT investigation of the adsorption of methyl on Rh(111). Surface Science, 2004, 558, 15-22.	0.8	20
54	Electronic excitation induced amorphization in titanate pyrochlores: an ab initio molecular dynamics study. Scientific Reports, 2015, 5, 8265.	1.6	20

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55	Pressure induced structural transformation in Gd₂Ti₂O₇and Gd₂Zr₂O₇. Journal of Physics Condensed Matter, 2011, 23, 035501.	0.7	19
56	Structural phase transitions in high-pressure wurtzite to rocksalt phase in GaN and SiC. Applied Physics Letters, 2008, 92, .	1.5	18
57	Theoretical prediction of long-range ferromagnetism in transition-metal atom-doped d⁰ dichalcogenide single layers SnS₂ and ZrS₂. Physical Chemistry Chemical Physics, 2016, 18, 25151-25160.	1.3	18
58	Impact of isovalent and aliovalent substitution on the mechanical and thermal properties of Gd2Zr2O7. Scientific Reports, 2017, 7, 6399.	1.6	17
59	Impact of point defects on electronic structure in Y2Ti2O7. RSC Advances, 2012, 2, 7235.	1.7	16
60	Ab initiomolecular dynamics simulations of threshold displacement energies in SrTiO₃. Journal of Physics Condensed Matter, 2013, 25, 485003.	0.7	16
61	Engineering the electronic and magnetic properties of d⁰ 2D dichalcogenide materials through vacancy doping and lattice strains. Physical Chemistry Chemical Physics, 2016, 18, 7163-7168.	1.3	16
62	Effects of surface defects on two-dimensional electron gas at NdAlO3/SrTiO3 interface. Scientific Reports, 2014, 4, 5477.	1.6	15
63	Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. Physical Chemistry Chemical Physics, 2020, 22, 22758-22767.	1.3	15
64	The thermal and electrical transport properties of layered LaCuOSe under high pressure. Journal of Alloys and Compounds, 2021, 861, 157984.	2.8	15
65	The effect of hydrogen on the mechanical properties of high entropy alloy TiZrHfMoNb: First-principles investigation. Journal of Alloys and Compounds, 2021, 879, 160482.	2.8	15
66	Ab initio calculations of structural and energetic properties of defects in gallium nitride. Journal of Applied Physics, 2008, 103, 123529.	1.1	14
67	High-electron-affinity oxide V2O5 enhances surface transfer doping on hydrogen-terminated diamond. Diamond and Related Materials, 2020, 108, 107865.	1.8	14
68	Stability of superconducting Nd0.8Sr0.2NiO2 thin films. Science China: Physics, Mechanics and Astronomy, 2022, 65, .	2.0	14
69	A Theoretical Simulation of the Radiation Responses of Si, Ge, and Si/Ge Superlattice to Low-Energy Irradiation. Nanoscale Research Letters, 2018, 13, 133.	3.1	13
70	Theoretical Combined Experimental Study of Unique He Behaviors in High-Entropy Alloys. Inorganic Chemistry, 2021, 60, 1388-1397.	1.9	12
71	Structural, electronic and magnetic properties of metalâ€“organic-framework perovskites [AmH][Mn(HCOO)3]: a first-principles study. RSC Advances, 2016, 6, 48779-48787.	1.7	11
72	Ab initio molecular dynamics simulation of low energy radiation responses of Î±-Al2O3. Scientific Reports, 2017, 7, 3621.	1.6	11

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73	A comparative study of the structural and optical properties of Si-doped GaAs under different ion irradiation. Optical Materials, 2021, 111, 110611.	1.7	11
74	Superior Hydrogen Sorption Kinetics of Ti0.20Zr0.20Hf0.20Nb0.40 High-Entropy Alloy. Metals, 2021, 11, 470.	1.0	11
75	The origin of anomalous hydrogen occupation in high entropy alloys. Journal of Materials Chemistry A, 2022, 10, 7228-7237.	5.2	11
76	Ab initiomolecular dynamics simulation of a pressure induced zinc blende to rocksalt phase transition in SiC. Journal of Physics Condensed Matter, 2009, 21, 245801.	0.7	10
77	Functionalized graphene nanoroads for quantum well device. Applied Physics Letters, 2011, 98, .	1.5	10
78	Enhanced electronic conductivity by controlled self-doping in pyrochlores. Physical Chemistry Chemical Physics, 2012, 14, 6556.	1.3	10
79	Structure and properties of rare earth silicates with the apatite structure at high pressure. Physics and Chemistry of Minerals, 2013, 40, 817-825.	0.3	9
80	Ab initio molecular dynamics simulation of the radiation damage effects of GaAs/AlGaAs superlattice. Journal of Nuclear Materials, 2019, 516, 228-237.	1.3	9
81	High-Dose Electron Radiation and Unexpected Room-Temperature Self-Healing of Epitaxial SiC Schottky Barrier Diodes. Nanomaterials, 2019, 9, 194.	1.9	9
82	Coexistence of epitaxial lattice rotation and twinning tilt induced by surface symmetry mismatch. Applied Physics Letters, 2014, 104, .	1.5	8
83	A DFT+U study on the thermodynamic properties of defective Gd2Zr2O7 pyrochlore. Journal of Nuclear Materials, 2020, 542, 152425.	1.3	8
84	Dehydrogenation: a simple route to modulate magnetism and spatial charge distribution of germanane. Journal of Materials Chemistry C, 2015, 3, 3128-3134.	2.7	7
85	First-principles study of point defects in U₃Si₂: effects on the mechanical and electronic properties. Physical Chemistry Chemical Physics, 2022, 24, 4287-4297.	1.3	7
86	Electronic Structure Calculations of A₂Ti₂O₇(A = Dy, Ho, and Y). Advances in Condensed Matter Physics, 2013, 2013, 1-8.	0.4	6
87	Nonlinear luminescence response of CaF2:Eu and YAlO3:Ce to single-ion excitation. Journal of Applied Physics, 2014, 115, 033108.	1.1	6
88	Effects of stacking periodicity on the electronic and optical properties of GaAs/AlAs superlattice: a first-principles study. Scientific Reports, 2020, 10, 4862.	1.6	6
89	Electronic structure regulation toward the improvement of the hydrogenation properties of TiZrHfMoNb high-entropy alloy. Journal of Alloys and Compounds, 2022, 905, 164150.	2.8	6
90	Effects of boron-nitride substrates on Stone-Wales defect formation in graphene: An ab initio molecular dynamics study. Applied Physics Letters, 2014, 104, 203106.	1.5	5

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91	First-Principles Study of Thermo-Physical Properties of Pu-Containing Gd2Zr2O7. Nanomaterials, 2019, 9, 196.	1.9	5
92	An AIMD+U simulation of low-energy displacement events in UO2. Journal of Nuclear Materials, 2020, 540, 152379.	1.3	5
93	Preliminary assessment of high-entropy alloys for tritium storage. Tungsten, 2021, 3, 119-130.	2.0	5
94	Effect of Copper Doping on Electronic Structure and Optical Absorption of Cd33Se33 Quantum Dots. Nanomaterials, 2021, 11, 2531.	1.9	5
95	A review of the properties, synthesis and applications of lanthanum copper oxychalcogenides. Journal Physics D: Applied Physics, 2022, 55, 273002.	1.3	5
96	Thermal Transport and Mechanical Properties of Layered Oxychalcogenides LaCuOX (X = S, Se, and Te). ACS Applied Energy Materials, 2022, 5, 6943-6951.	2.5	5
97	Ab initio molecular dynamics simulation of pressure-induced phase transformation in BeO. Journal of Materials Science, 2011, 46, 6408-6415.	1.7	4
98	Structural Features and Photoelectric Properties of Si-Doped GaAs under Gamma Irradiation. Nanomaterials, 2020, 10, 340.	1.9	4
99	A First-Principles Study of Hydrogen Desorption from High Entropy Alloy TiZrVMoNb Hydride Surface. Metals, 2021, 11, 553.	1.0	4
100	Effect of S adsorption on magnetic Co(0001) surface: a DFT study. European Physical Journal B, 2008, 61, 319-324.	0.6	3
101	ADSORPTION OF Li ON Mo(110) SURFACE: A FIRST-PRINCIPLES STUDY. Surface Review and Letters, 2009, 16, 589-597.	0.5	3
102	Formation and migration of vacancy defects in GeSe and SnSe. Journal of Physics B: Atomic, Molecular and Optical Physics, 0, , .	0.6	3
103	First-principles study of stability of point defects and their effects on electronic properties of GaAs/AlGaAs superlattice. Chinese Physics B, 2022, 31, 036104.	0.7	3
104	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, .	0.9	3
105	An abnormal incorporation behavior of Th in Gd 2 Zr 2 O 7 : A firstâ€principles study. Journal of the American Ceramic Society, 2020, 103, 1846-1853.	1.9	2
106	Defect formation and its effect on the thermodynamic properties of Pu₂Zr₂O₇ pyrochlore: a firstâ€principles study. Journal of the American Ceramic Society, 2021, 104, 2301-2312.	1.9	2
107	First-principles study of fission products Xe and Cs behaviors in U₃Si₂. Journal of Physics Condensed Matter, 2022, 34, 165702.	0.7	2
108	Effects of temperature and energy on the radiation response of GaAs/AlAs and GaAs/AlGaAs superlattices. Radiation Physics and Chemistry, 2020, 174, 108983.	1.4	1

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109	A Comparative Study of Electron Radiation Responses of Pu2Zr2O7 and La2Zr2O7: An abinitio Molecular Dynamics Study. Materials, 2021, 14, 1516.	1.3	1
110	Structural and electronic properties of 0.5 ML sulfur adsorbed on the GaP(001) surface. Journal of Materials Science, 2011, 46, 1635-1639.	1.7	0
111	Electrostatic Asymmetry of Wurtzite Nanocrystals and Resulting Photocatalytic Properties. Journal of Physical Chemistry C, 2022, 126, 4751-4761.	1.5	0