Yifang Ouyang

List of Publications by Citations

101 papers	1,435 citations	21 h-index	32 g-index
104 ext. papers	1,688 ext. citations	3.4 avg, IF	4.37 L-index

#	Paper	IF	Citations
101	A thermodynamic description of the Al-Fe-Si system over the whole composition and temperature ranges via a hybrid approach of CALPHAD and key experiments. *Intermetallics*, **2008**, 16, 554-570	3.5	149
100	Phase stability of magnesium-rare earth binary systems from first-principles calculations. *Journal of Alloys and Compounds*, **2011**, 509, 6899-6907	5.7	47
99	Formation enthalpies of Fe-Al-RE ternary alloys calculated with a geometric model and Miedema's theory. *Journal of Alloys and Compounds*, **2006**, 416, 148-154	5.7	46
98	Structural evolution of mechanically alloyed nanocrystalline FeAl intermetallics. *Journal of Alloys and Compounds*, **2008**, 455, 207-209	5.7	45
97	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers via biaxial straining. *Nanoscale*, **2019**, 11, 2335-2342	7.7	42
96	Elastic constants of B2-MgRE (RE= Sc, Y, La-Lu) calculated with first-principles. *Solid State Communications*, **2008**, 148, 314-318	1.6	42
95	Calculation of the thermodynamic properties of B2 AlRE (RE=Sc, Y, La, Ce-Lu). *Physica B: Condensed Matter*, **2007**, 399, 27-32	2.8	39
94	Ab initio calculation of the total energy and elastic properties of Laves phase C15 Al2RE (RE=Sc, Y, La, Ce-Lu). *Computational Materials Science*, **2008**, 44, 392-399	3.2	37
93	Distinct green electroluminescence from lead-free CsCuBr halide micro-crosses. *Chemical Communications*, **2019**, 55, 4554-4557	5.8	33
92	Thermodynamic modeling of the V-Si system supported by key experiments. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2008**, 32, 320-325	1.9	33
91	Ab initio calculations of mechanical and thermodynamic properties for the B2-based AlRE. *Computational Materials Science*, **2007**, 40, 226-233	3.2	33
90	Enthalpies of formation for the Al-Cu-Ni-Zr quaternary alloys calculated via a combined approach of geometric model and Miedema theory. *Journal of Alloys and Compounds*, **2006**, 420, 175-181	5.7	31
89	Highly-efficient all-inorganic lead-free 1D CsCu2I3 single crystal for white-light emitting diodes and UV photodetection. *Nano Energy*, **2021**, 81, 105570	17.1	31
88	Density-functional theory study of Aln and Aln-1Mg (n = 2-17) clusters. *Computational and Theoretical Chemistry*, **2012**, 984, 68-75	2	30
87	Machine learning reveals the importance of the formation enthalpy and atom-size difference in forming phases of high entropy alloys. *Materials and Design*, **2020**, 193, 108835	8.1	29
86	First-principles calculations of the thermodynamic and elastic properties of the L12-based Al3RE (RE = Sc, Y, La-Lu). *International Journal of Materials Research*, **2008**, 99, 582-588	0.5	29
85	The formation and crystallization of amorphous Al65Fe20Zr15. *Journal of Non-Crystalline Solids*, **2008**, 354, 5555-5558	3.9	28

84	Crystallization study of amorphous Al82Fe5Ni5Ce8 alloy. *Journal of Alloys and Compounds*, **2008**, 454, 359-363	5.7	28
83	Thermodynamic and physical properties of FeAl and Fe3Al: an atomistic study by EAM simulation. *Physica B: Condensed Matter*, **2012**, 407, 4530-4536	2.8	27
82	Thermodynamic modeling of the CuMn system supported by key experiments. *Journal of Alloys and Compounds*, **2008**, 457, 233-238	5.7	24
81	Molecular dynamics simulation of diffusion bonding of AlCu interface. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 065013	2	22
80	Enhanced ultraviolet electroluminescence and spectral narrowing from ZnO quantum dots/GaN heterojunction diodes by using high-k HfO2 electron blocking layer. *Applied Physics Letters*, **2014**, 105, 063505	3.4	20
79	Strengthening by the percolating intergranular eutectic in an HPDC MgCe alloy. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2014**, 599, 204-211	5.3	20
78	Structure and thermodynamics of the key precipitated phases in the AlMgSi alloys from first-principles calculations. *Journal of Materials Science*, **2011**, 46, 7839-7849	4.3	20
77	Extended solid solubility for Al-W binary system by mechanical alloying. *Science in China Series A: Mathematics*, **2000**, 43, 180-184		20
76	Structure, elastic and thermodynamic properties of the NiP system from first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2011**, 35, 284-291	1.9	19
75	Structural, electronic and elastic properties of V5Si3 phases from first-principles calculations. *Computational Materials Science*, **2012**, 53, 169-174	3.2	18
74	Thermodynamic optimization of the CuNd system. *Journal of Alloys and Compounds*, **2011**, 509, 2679-2683	5.7	18
73	The effect of Ti atom on hydrogenation of Al(111) surface: First-principles studies. *International Journal of Hydrogen Energy*, **2010**, 35, 609-613	6.7	18
72	First-principles calculations of mechanical and thermodynamic properties of the Laves C15-Mg2RE (RE = La, Ce, Pr, Nd, Pm, Sm, Gd). *Computational Materials Science*, **2009**, 47, 297-301	3.2	17
71	First-principles study of binary special quasirandom structures for the AlCu, AlSi, CuSi, and MgSi systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 769-773	1.9	16
70	The structural stability, elastic constants and electronic structure of AlSr intermetallics by first-principles calculations. *Physica B: Condensed Matter*, **2011**, 406, 3681-3686	2.8	16
69	Contribution on the phase equilibria in ZrNbFe system. *Journal of Nuclear Materials*, **2015**, 466, 627-633	3.3	15
68	Analytic embedded-atom potentials for bcc metals: application to calculating the thermodynamic data of bcc alloys. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1994**, 192, 79-86	2.3	15
67	An experimental study on the interdiffusion behaviors and mechanical properties of Ni-Zr system. *Journal of Alloys and Compounds*, **2018**, 752, 412-419	5.7	14

66	Interdiffusion behaviors and mechanical properties of Cu-Zr system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2018**, 61, 92-97	1.9	14
65	First-principles investigations of elastic, electronic and thermodynamic properties of Al12X (X=Mo, W and Re). *Intermetallics*, **2012**, 24, 15-21	3.5	13
64	Nano-amorphous (FeAl)1-xZrx alloys prepared by mechanical alloying. *Journal of Alloys and Compounds*, **2006**, 421, 314-318	5.7	13
63	First principle study of AlX (X=3d, 4d, 5d elements and Lu) dimer. *Journal of Chemical Physics*, **2008**, 128, 074305	3.9	12
62	Diffusivities and atomic mobilities for fcc Cu-Ni-Sn alloys. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2017**, 59, 84-89	1.9	11
61	First-principles investigation of the thermo-physical properties of Ca3Si4. *Journal of Solid State Chemistry*, **2012**, 194, 179-187	3.3	11
60	Elastic, phonon and thermodynamic properties of Mg-Ca compounds from first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2012**, 37, 137-144	1.9	11
59	The mechanical, electronic structure and thermodynamic properties of B2-based AgRE studied from first-principles. *Physica Scripta*, **2011**, 83, 045301	2.6	11
58	First-principles calculations of elastic constants of DO3-Mg3RE (RE = Sc, Y, La, Ce, Lu). *Physica Scripta*, **2008**, 78, 065601	2.6	11
57	Interactions between Er dopant and intrinsic point defects of ZnO: a first-principles study. *Materials Research Express*, **2017**, 4, 035903	1.7	10
56	Phase stability, thermodynamic and mechanical properties of AlZr2, FeZr2 and Al2FeZr6 from first-principles calculations. *Journal of Nuclear Materials*, **2013**, 440, 6-10	3.3	10
55	Formation enthalpies of Al-Fe-Zr-Nd system calculated by using geometric and Miedema's models. *Physica B: Condensed Matter*, **2015**, 463, 82-87	2.8	10
54	Phase equilibria of the Ni-Ti-Ta system at 927°C. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2007**, 448, 210-215	5.3	10
53	Highly Efficient Polarized GeS/MoSe2 van der Waals Heterostructure for Water Splitting from Ultraviolet to Near-Infrared Light. *Physica Status Solidi - Rapid Research Letters*, **2020**, 14, 1900582	2.5	10
52	Investigation of diffusion behavior and mechanical properties of Mg-Zn system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2019**, 65, 204-211	1.9	9
51	(FeAl3)1-xZrx amorphous alloys prepared by mechanical alloying. *Physica B: Condensed Matter*, **2007**, 391, 380-384	2.8	9
50	Preparation of iron-tungsten-boron alloy deposits by electroless plating. *Metal Finishing*, **1996**, 94, 31-35		9
49	Crystallization of Al2FeZr6 Amorphous Alloy Prepared by Mechanical Alloying. *Materials Transactions*, **2006**, 47, 388-391	1.3	8

48	Mechanical Alloying of Fe25Al75−xTix Mixed Powders. *Materials Transactions*, **2004**, 45, 1774-1777	1.3	8
47	Low-voltage multicolor electroluminescence from all-inorganic carbon dots/Si-heterostructured light-emitting diodes. *Journal of Materials Science*, **2019**, 54, 8492-8503	4.3	7
46	Boosted electroluminescence of perovskite light-emitting diodes by pinhole passivation with insulating polymer. *Journal Physics D: Applied Physics*, **2018**, 51, 405103	3	7
45	Density functional study of 3d-transition metal aluminides. *Computational and Theoretical Chemistry*, **2009**, 905, 106-112		7
44	Development of a modified embedded atom method for bcc transition metals. *Journal of Physics Condensed Matter*, **2003**, 15, 8917-8926	1.8	7
43	Diffusional behaviors and mechanical properties of Cu□n system. *Journal of Alloys and Compounds*, **2020**, 812, 152141	5.7	7
42	Toward near-white electroluminescence with enhanced blue emission from carbon dots in PEDOT:PSS/ZnO organic/inorganic hybrid heterojunctions. *Journal of Luminescence*, **2020**, 224, 117230	3.8	6
41	An interatomic potential for simulation of defects and phase change of zirconium. *Computational Materials Science*, **2018**, 147, 7-17	3.2	6
40	Surface energy and surface self-diffusion of Al calculated by embedded atom method. *Physica B: Condensed Matter*, **2013**, 422, 51-55	2.8	6
39	Atomic parameter model for the solid solubilities in binary transition metal based alloys. *Indian Journal of Physics*, **2011**, 85, 261-270	1.4	6
38	First-principles calculations of elastic and thermo-physical properties of Al, Mg and rare earth lanthanide elements. *Physica B: Condensed Matter*, **2009**, 404, 2299-2304	2.8	6
37	Strain Enhanced Visible□Ultraviolet Absorption of Blue Phosphorene/MoX2 (X = S,Se) Heterolayers. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800659	2.5	5
36	Experimental Investigation on Phase Equilibria of Al-Fe-Y System at 773 K. *Journal of Phase Equilibria and Diffusion*, **2014**, 35, 256-261	1	5
35	Investigation of thermophysical, electronic and lattice dynamic properties for CaX2Si2 (X=Ni,Zn,Cu,Ag,Au) via first-principles calculations. *Computational Materials Science*, **2015**, 102, 167-173	3.2	5
34	Experimental investigation on phase equilibria of Ce-Sn-Zn system at 400 □C. *Journal of Rare Earths*, **2012**, 30, 916-922	3.7	5
33	First-principles investigation of the mechanical, electronic and thermophysical properties of Q-phase in Al□Mg□Si□Cu alloys. *Computational Materials Science*, **2013**, 67, 334-340	3.2	5
32	The elastic constants for Fe3AlX(X=B, C and N) with anti-perovskite structure. *Physica Scripta*, **2009**, 80, 055603	2.6	5
31	Electronic calculation of Mn3AlN with anti-perovskite structure. *Computational Materials Science*, **2008**, 44, 97-101	3.2	5

30	Theoretical study of spectroscopic parameters of alkali -Al and alkaline earth-Al dimers. *Theoretical Chemistry Accounts*, **2008**, 121, 165-172	1.9	5
29	Phase Stability and Mechanical Properties of Al□e□RE via First-Principle Calculations. *Materials*, **2019**, 12,	3.5	4
28	Enhanced electroluminescence from n-ZnO NCs/n-Si isotype heterojunctions by using i-NiO as electron blocking layer. *Journal of Luminescence*, **2018**, 204, 5-9	3.8	4
27	Experimental Investigation of the Al-Fe-Nd System at 773 K. *Journal of Phase Equilibria and Diffusion*, **2014**, 35, 86-92	1	4
26	Toward near-white-light electroluminescence from n-ZnO nanocrystals/n-Si isotype heterojunctions via an AZO spectral scissor. *Optics Express*, **2017**, 25, 19004-19012	3.3	4
25	Experimental Investigation of the Al-Fe-Gd System at 773 K. *Journal of Phase Equilibria and Diffusion*, **2013**, 34, 116-121	1	3
24	Elastic constants and thermophysical properties of Al□MgSi alloys from first-principles calculations. *International Journal of Materials Research*, **2010**, 101, 1392-1397	0.5	3
23	Structure and stability of Al□e□rCe cluster: density functional study. *Theoretical Chemistry Accounts*, **2010**, 127, 651-659	1.9	3
22	The formation and crystallization for amorphous AlFeZr4 prepared by mechanical alloying. *Physica B: Condensed Matter*, **2010**, 405, 2005-2008	2.8	3
21	Diffusional behaviors and mechanical properties of Ni-Zn system. *Journal of Alloys and Compounds*, **2021**, 881, 160581	5.7	3
20	Improving and manipulating green-light electroluminescence in solution-processed ZnO nanocrystals via erbium doping. *Journal of Luminescence*, **2019**, 213, 127-132	3.8	2
19	The Isothermal Section of the Zr-Sn-Cu Ternary System at 700 °C. *Journal of Phase Equilibria and Diffusion*, **2018**, 39, 196-203	1	2
18	Exploring phase stability, electronic and mechanical properties of CePb intermetallic compounds using first-principles calculations. *Journal of Solid State Chemistry*, **2016**, 237, 385-393	3.3	2
17	Lattice dynamics properties of XAs (X=Al, Ga and In) with zinc-blende structure from first-principle calculations. *Journal of Physics and Chemistry of Solids*, **2012**, 73, 1034-1039	3.9	2
16	Size and composition dependence of melting temperature of binary nanoparticles. *Science China: Physics, Mechanics and Astronomy*, **2011**, 54, 897-900	3.6	2
15	The atomic parameter model for the fifth and sixth transition metal quasicrystal alloys (Mc=0.5) **2009**, 52, 1593-1600		2
14	Model Equations for Solid Solubilities in Binary Non-Transition Metal Based Alloys. *Materials Transactions, JIM*, **1997**, 38, 589-594		2
13	The compositional range of amorphous phase formation and thermal stability of Al90□Fe5Ni5Cex. *Journal of Alloys and Compounds*, **2008**, 460, 309-313	5.7	2

12	Two-dimensional polarized MoTe/GeS heterojunction with an intrinsic electric field for photocatalytic water-splitting.. *RSC Advances*, **2021**, 11, 34048-34058	3.7	2
11	Codoping Er-N to Suppress Self-Compensation Donors for Stable p-Type Zinc Oxide. *Advanced Theory and Simulations*, **2019**, 2, 1800133	3.5	2
10	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. *Journal of Materials Science*, **2019**, 54, 10284-10296	4.3	1
9	The effect of Al content on the structural, mechanical, and thermal properties of B2-FeAl and D03-Fe3Al from atomistic study. *Materials Research Express*, **2018**, 5, 026512	1.7	1
8	The effect of grain boundary energy on the amorphous forming composition range of Zr□Fe□Al ternary system. *Journal of Non-Crystalline Solids*, **2016**, 432, 277-284	3.9	1
7	The electronic, mechanical and lattice dynamic properties of TiSiY from first-principles calculations. *Computational Materials Science*, **2012**, 65, 485-489	3.2	1
6	Suggest a new approach to fabricate AlFe2B2. *Computational Materials Science*, **2020**, 171, 109239	3.2	1
5	Molecular dynamics simulation of diffusion for Ni□r interface. *International Journal of Modern Physics B*, **2020**, 34, 2050217	1.1	1
4	Interdiffusion behaviors and mechanical properties of Zn□r system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2021**, 74, 102308	1.9	1
3	Isothermal Section of the Al-Zn-RE (RE = Ho, Er) Systems at 450 □C. *Journal of Phase Equilibria and Diffusion*, **2016**, 37, 658-663	1	0
2	Interdiffusion behaviors and mechanical properties in BCC Zr-rich Zr□Nb□a system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2022**, 77, 102410	1.9	0
1	Interdiffusion behaviors and mechanical properties of Zr-X (X Nb, Ta, Hf) binary systems. *Journal of Alloys and Compounds*, **2022**, 910, 164910	5.7	0