Yifang Ouyang

List of Publications by Year
in descending order

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102 papers	1,962 citations	279798 23 h-index	315739 38 g-index
104 all docs	104 docs citations	104 times ranked	1731 citing authors

#	Article	IF	Citations
1	A thermodynamic description of the Alâ€“Feâ€“Si system over the whole composition and temperature ranges via a hybrid approach of CALPHAD and key experiments. Intermetallics, 2008, 16, 554-570.	3.9	177
2	Highly-efficient all-inorganic lead-free 1D CsCu2I3 single crystal for white-light emitting diodes and UV photodetection. Nano Energy, 2021, 81, 105570.	16.0	100
3	Enhanced photocatalytic activity for water splitting of blue-phase GeS and GeSe monolayers via biaxial straining. Nanoscale, 2019, 11, 2335-2342.	5.6	80
4	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.	7.0	68
5	Phase stability of magnesium-rare earth binary systems from first-principles calculations. Journal of Alloys and Compounds, 2011, 509, 6899-6907.	5.5	59
6	Elastic constants of B2-MgRE (REÂ= ÂSc, Y, Laâ€“Lu) calculated with first-principles. Solid State Communications, 2008, 148, 314-318.	1.9	54
7	Formation enthalpies of Feâ€“Alâ€“RE ternary alloys calculated with a geometric model and Miedema's theory. Journal of Alloys and Compounds, 2006, 416, 148-154.	5.5	53
8	Distinct green electroluminescence from lead-free CsCuBr₂ halide micro-crosses. Chemical Communications, 2019, 55, 4554-4557.	4.1	52
9	Structural evolution of mechanically alloyed nanocrystalline FeAl intermetallics. Journal of Alloys and Compounds, 2008, 455, 207-209.	5.5	50
10	Calculation of the thermodynamic properties of B2 AlRE (RE=Sc, Y, La, Ceâ€“Lu). Physica B: Condensed Matter, 2007, 399, 27-32.	2.7	43
11	Ab initio calculation of the total energy and elastic properties of Laves phase C15 Al2RE (RE=Sc, Y, La,) Tj ETQq1 1 0.784314 rgBT /Ov	3.0	43
12	Thermodynamic modeling of the Vâ€“Si system supported by key experiments. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 320-325.	1.6	40
13	Enthalpies of formation for the Alâ€“Cuâ€“Niâ€“Zr quaternary alloys calculated via a combined approach of geometric model and Miedema theory. Journal of Alloys and Compounds, 2006, 420, 175-181.	5.5	39
14	Ab initio calculations of mechanical and thermodynamic properties for the B2-based AlRE. Computational Materials Science, 2007, 40, 226-233.	3.0	38
15	First-principles calculations of the thermodynamic and elastic properties of the L1₂-based Al₃RE (RE = Sc, Y, Laâ€“Lu). International Journal of Materials Research, 2008, 99, 582-588.	0.3	35
16	Molecular dynamics simulation of diffusion bonding of Alâ€“Cu interface. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 065013.	2.0	35
17	The formation and crystallization of amorphous Al65Fe20Zr15. Journal of Non-Crystalline Solids, 2008, 354, 5555-5558.	3.1	33
18	Density-functional theory study of Aln and Alnâ^'1Mg (n=2â€“17) clusters. Computational and Theoretical Chemistry, 2012, 984, 68-75.	2.5	33

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19	Thermodynamic and physical properties of FeAl and Fe3Al: an atomistic study by EAM simulation. Physica B: Condensed Matter, 2012, 407, 4530-4536.	2.7	31
20	Crystallization study of amorphous Al82Fe5Ni5Ce8 alloy. Journal of Alloys and Compounds, 2008, 454, 359-363.	5.5	28
21	Thermodynamic modeling of the Cuâ€“Mn system supported by key experiments. Journal of Alloys and Compounds, 2008, 457, 233-238.	5.5	27
22	Structure and thermodynamics of the key precipitated phases in the Alâ€“Mgâ€“Si alloys from first-principles calculations. Journal of Materials Science, 2011, 46, 7839-7849.	3.7	26
23	Structure, elastic and thermodynamic properties of the Niâ€“P system from first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 284-291.	1.6	25
24	An experimental study on the interdiffusion behaviors and mechanical properties of Ni-Zr system. Journal of Alloys and Compounds, 2018, 752, 412-419.	5.5	24
25	Investigation of diffusion behavior and mechanical properties of Mg-Zn system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 65, 204-211.	1.6	24
26	Extended solid solubility for Al-W binary system by mechanical alloying. Science in China Series A: Mathematics, 2000, 43, 180-184.	0.5	23
27	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.	3.0	23
28	Strengthening by the percolating intergranular eutectic in an HPDC Mgâ€“Ce alloy. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2014, 599, 204-211.	5.6	23
29	Diffusional behaviors and mechanical properties of Cuâ€“Zn system. Journal of Alloys and Compounds, 2020, 812, 152141.	5.5	23
30	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.	3.3	22
31	Contribution on the phase equilibria in Zrâ€“Nbâ€“Fe system. Journal of Nuclear Materials, 2015, 466, 627-633.	2.7	21
32	Thermodynamic optimization of the Cuâ€“Nd system. Journal of Alloys and Compounds, 2011, 509, 2679-2683.	5.5	20
33	Structural, electronic and elastic properties of V5Si3 phases from first-principles calculations. Computational Materials Science, 2012, 53, 169-174.	3.0	20
34	Interdiffusion behaviors and mechanical properties of Cu-Zr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 92-97.	1.6	19
35	The effect of Ti atom on hydrogenation of Al(111) surface: First-principles studies. International Journal of Hydrogen Energy, 2010, 35, 609-613.	7.1	18
36	The structural stability, elastic constants and electronic structure of Alâ€“Sr intermetallics by first-principles calculations. Physica B: Condensed Matter, 2011, 406, 3681-3686.	2.7	18

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37	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.	2.1	17
38	First-principles study of binary special quasirandom structures for the Alâ€“Cu, Alâ€“Si, Cuâ€“Si, and Mgâ€“Si systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 769-773.	1.6	17
39	First-principles investigations of elastic, electronic and thermodynamic properties of Al12X (XÂ=ÂMo, W) Tj ETQq1 1 0.784314 rgBT /Ov	3.9	17
40	Diffusivities and atomic mobilities for fcc Cuâ€“Niâ€“Sn alloys. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 59, 84-89.	1.6	17
41	First principle study of AlX (X=3d,4d,5d elements and Lu) dimer. Journal of Chemical Physics, 2008, 128, 074305.	3.0	15
42	Nano-amorphous (FeAl)1â^'xZrx alloys prepared by mechanical alloying. Journal of Alloys and Compounds, 2006, 421, 314-318.	5.5	14
43	Highly Efficient Polarized GeS/MoSe₂ van der Waals Heterostructure for Water Splitting from Ultraviolet to Nearâ€Infrared Light. Physica Status Solidi - Rapid Research Letters, 2020, 14, 1900582.	2.4	14
44	Diffusional behaviors and mechanical properties of Ni-Zn system. Journal of Alloys and Compounds, 2021, 881, 160581.	5.5	14
45	Phase equilibria of the Niâ€“Tiâ€“Ta system at 927Â°C. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2007, 448, 210-215.	5.6	13
46	First-principles calculations of elastic constants of DO₃-Mg₃RE (RE = Sc, Y, La,) Tj ETQq0 0 0 rgBT /Overlock 1	2.5	13
47	First-principles investigation of the thermo-physical properties of Ca3Si4. Journal of Solid State Chemistry, 2012, 194, 179-187.	2.9	13
48	Phase stability, thermodynamic and mechanical properties of AlZr2, FeZr2 and Al2FeZr6 from first-principles calculations. Journal of Nuclear Materials, 2013, 440, 6-10.	2.7	13
49	The mechanical, electronic structure and thermodynamic properties of B2-based AgRE studied from first-principles. Physica Scripta, 2011, 83, 045301.	2.5	12
50	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.	2.7	11
51	Elastic, phonon and thermodynamic properties of Mgâ€“Ga compounds from first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2012, 37, 137-144.	1.6	11
52	Formation enthalpies of Alâ€“Feâ€“Zrâ€“Nd system calculated by using geometric and Miedema's models. Physica B: Condensed Matter, 2015, 463, 82-87.	2.7	11
53	Exploring phase stability, electronic and mechanical properties of Ceâ€“Pb intermetallic compounds using first-principles calculations. Journal of Solid State Chemistry, 2016, 237, 385-393.	2.9	11
54	Interactions between Er dopant and intrinsic point defects of ZnO: a first-principles study. Materials Research Express, 2017, 4, 035903.	1.6	11

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55	Two-dimensional polarized MoTe₂/GeS heterojunction with an intrinsic electric field for photocatalytic water-splitting. RSC Advances, 2021, 11, 34048-34058.	3.6	11
56	(FeAl3)1â^'xZrx amorphous alloys prepared by mechanical alloying. Physica B: Condensed Matter, 2007, 391, 380-384.	2.7	10
57	An interatomic potential for simulation of defects and phase change of zirconium. Computational Materials Science, 2018, 147, 7-17.	3.0	10
58	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.	3.1	10
59	Preparation of iron-tungsten-boron alloy deposits by electroless plating. Metal Finishing, 1996, 94, 31-35.	0.0	9
60	Crystallization of Al₂FeZr₆ Amorphous Alloy Prepared by Mechanical Alloying. Materials Transactions, 2006, 47, 388-391.	1.2	9
61	Low-voltage multicolor electroluminescence from all-inorganic carbon dots/Si-heterostructured light-emitting diodes. Journal of Materials Science, 2019, 54, 8492-8503.	3.7	9
62	Suggest a new approach to fabricate AlFe2B2. Computational Materials Science, 2020, 171, 109239.	3.0	9
63	Interdiffusion behaviors and mechanical properties of Znâ€“Cr system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102308.	1.6	9
64	Development of a modified embedded atom method for bcc transition metals. Journal of Physics Condensed Matter, 2003, 15, 8917-8926.	1.8	8
65	Mechanical Alloying of Fe₂₅Al_{75−x}Ti_x Mixed Powders. Materials Transactions, 2004, 45, 1774-1777.	1.2	8
66	Density functional study of 3d-transition metal aluminides. Computational and Theoretical Chemistry, 2009, 905, 106-112.	1.5	8
67	Atomic parameter model for the solid solubilities in binary transition metal based alloys. Indian Journal of Physics, 2011, 85, 261-270.	1.8	8
68	Surface energy and surface self-diffusion of Al calculated by embedded atom method. Physica B: Condensed Matter, 2013, 422, 51-55.	2.7	8
69	First-principles investigation of the mechanical, electronic and thermophysical properties of Q-phase in Alâ€“Mgâ€“Siâ€“Cu alloys. Computational Materials Science, 2013, 67, 334-340.	3.0	8
70	Experimental Investigation on Phase Equilibria of Al-Fe-Y System at 773ÂK. Journal of Phase Equilibria and Diffusion, 2014, 35, 256-261.	1.4	8
71	Boosted electroluminescence of perovskite light-emitting diodes by pinhole passivation with insulating polymer. Journal Physics D: Applied Physics, 2018, 51, 405103.	2.8	8
72	The elastic constants for Fe₃AlX (X=B, C and N) with anti-perovskite structure. Physica Scripta, 2009, 80, 055603.	2.5	7

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73	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.	3.0	7
74	Toward near-white-light electroluminescence from n-ZnO nanocrystals/n-Si isotype heterojunctions via an AZO spectral scissor. Optics Express, 2017, 25, 19004.	3.4	7
75	Interdiffusion behaviors and mechanical properties in BCC Zr-rich Zrâ€“Nbâ€“Ta system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102410.	1.6	7
76	Theoretical study of spectroscopic parameters of alkali -Al and alkaline earth-Al dimers. Theoretical Chemistry Accounts, 2008, 121, 165-172.	1.4	6
77	Experimental investigation on phase equilibria of Ce-Sn-Zn system at 400 Â°C. Journal of Rare Earths, 2012, 30, 916-922.	4.8	6
78	Electronic calculation of Mn3AlN with anti-perovskite structure. Computational Materials Science, 2008, 44, 97-101.	3.0	5
79	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.	3.1	5
80	Strain Enhanced Visibleâ€“Ultraviolet Absorption of Blue Phosphorene/MoX 2 (Xâ€‰=â€‰S,Se) Heterolayers. Physica Status Solidi - Rapid Research Letters, 2019, 13, 1800659.	2.4	5
81	Interdiffusion behaviors and mechanical properties of Zr-X (X Nb, Ta, Hf) binary systems. Journal of Alloys and Compounds, 2022, 910, 164910.	5.5	5
82	The compositional range of amorphous phase formation and thermal stability of Al90â^'xFe5Ni5Cex. Journal of Alloys and Compounds, 2008, 460, 309-313.	5.5	4
83	The atomic parameter model for the fifth and sixth transition metal quasicrystal alloys (Mc=0.5). Science in China Series G: Physics, Mechanics and Astronomy, 2009, 52, 1593-1600.	0.2	4
84	The formation and crystallization for amorphous AlFeZr4 prepared by mechanical alloying. Physica B: Condensed Matter, 2010, 405, 2005-2008.	2.7	4
85	Experimental Investigation of the Al-Fe-Nd System at 773ÂK. Journal of Phase Equilibria and Diffusion, 2014, 35, 86-92.	1.4	4
86	Improving and manipulating green-light electroluminescence in solution-processed ZnO nanocrystals via erbium doping. Journal of Luminescence, 2019, 213, 127-132.	3.1	4
87	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. Journal of Materials Science, 2019, 54, 10284-10296.	3.7	4
88	Phase Stability and Mechanical Properties of Al8Fe4RE via First-Principle Calculations. Materials, 2019, 12, 701.	2.9	4
89	Molecular dynamics simulation of diffusion for Niâ€“Zr interface. International Journal of Modern Physics B, 2020, 34, 2050217.	2.0	4
90	Structure and stability of Alâ€“Feâ€“Zrâ€“Ce cluster: density functional study. Theoretical Chemistry Accounts, 2010, 127, 651-659.	1.4	3

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91	Elastic constants and thermophysical properties of Alâ€“Mgâ€“Si alloys from first-principles calculations. International Journal of Materials Research, 2010, 101, 1392-1397.	0.3	3
92	Experimental Investigation of the Al-Fe-Gd System at 773ÂK. Journal of Phase Equilibria and Diffusion, 2013, 34, 116-121.	1.4	3
93	The effect of grain boundary energy on the amorphous forming composition range of Zrâ€“Feâ€“Al ternary system. Journal of Non-Crystalline Solids, 2016, 432, 277-284.	3.1	3
94	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.	1.6	3
95	Model Equations for Solid Solubilities in Binary Non-Transition Metal Based Alloys. Materials Transactions, JIM, 1997, 38, 589-594.	0.9	2
96	Size and composition dependence of melting temperature of binary nanoparticles. Science China: Physics, Mechanics and Astronomy, 2011, 54, 897-900.	5.1	2
97	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.	4.0	2
98	Isothermal Section of theÂAl-Zn-RE (REÂ=ÂHo, Er) Systems at 450ÂÂ°C. Journal of Phase Equilibria and Diffusion, 2016, 37, 658-663.	1.4	2
99	The Isothermal Section of the Zr-Sn-Cu Ternary System at 700ÂÂ°C. Journal of Phase Equilibria and Diffusion, 2018, 39, 196-203.	1.4	2
100	Codoping Erâ€N to Suppress Selfâ€Compensation Donors for Stablepâ€Type Zinc Oxide. Advanced Theory and Simulations, 2019, 2, 1800133.	2.8	2
101	The electronic, mechanical and lattice dynamic properties of TiSiY from first-principles calculations. Computational Materials Science, 2012, 65, 485-489.	3.0	1
102	Polarization Electric Field in 2D Polar Monolayer Silicon Monochalcogenides SiX (Xâ€‰=â€‰S, Se) as Potential Photocatalysts for Water Splitting. Physica Status Solidi - Rapid Research Letters, 2023, 17, .	2.4	1