Ruifeng Zhang

List of Publications by Year in Descending Order

163 papers	5,577 citations	43 h-index	69 g-index
164 ext. papers	6,561 ext. citations	6.5 avg, IF	6.06 L-index

#	Paper	IF	Citations
163	Regulating oxygen covalent electron localization to enhance anionic redox reversibility of lithium-rich layered oxide cathodes. *Energy Storage Materials*, **2022**, 46, 512-522	19.4	5
162	MAELAS 2.0: A new version of a computer program for the calculation of magneto-elastic properties. *Computer Physics Communications*, **2022**, 271, 108197	4.2	1
161	Electrochemical CO reduction to ethylene by ultrathin CuO nanoplate arrays.. *Nature Communications*, **2022**, 13, 1877	17.4	11
160	Heterogeneous interface-boosted zinc storage of H2V3O8 nanowire/Ti3C2Tx MXene composite toward high-rate and long cycle lifespan aqueous zinc-ion batteries. *Energy Storage Materials*, **2022**, 50, 63-74	19.4	5
159	EAPOTc: An integrated empirical interatomic potential optimization platform for compound solids. *Computational Materials Science*, **2022**, 211, 111551	3.2	
158	Effect of void morphology on void facilitated plasticity in irradiated Cu/Nb metallic nanolayered composites. *Journal of Nuclear Materials*, **2021**, 153380	3.3	2
157	SPaMD studio: An integrated platform for atomistic modeling, simulation, analysis, and visualization. *Computational Materials Science*, **2021**, 111027	3.2	1
156	An improved electrochemical model for strain dependent electrochemical polarization and corrosion kinetics. *Materials and Design*, **2021**, 202, 109555	8.1	2
155	Revealing the Pressure-Induced Softening/Weakening Mechanism in Representative Covalent Materials. *Chinese Physics Letters*, **2021**, 38, 056101	1.8	
154	Cooperative roles of stacking fault energies on dislocation nucleation at bimetal interface through tunable potentials. *Computational Materials Science*, **2021**, 193, 110416	3.2	1
153	MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach. *Computer Physics Communications*, **2021**, 264, 107964	4.2	2
152	Giant heterogeneous magnetostriction induced by charge accumulation-mediated nanoinclusion formation in dual-phase nanostructured systems. *Acta Materialia*, **2021**, 213, 116975	8.4	9
151	Faceted Kurdjumov-Sachs interface-induced slip continuity in the eutectic high-entropy alloy, AlCoCrFeNi2.1. *Journal of Materials Science and Technology*, **2021**, 65, 216-227	9.1	26
150	Decoupled Redox Catalytic Hydrogen Production with a Robust Electrolyte-Borne Electron and Proton Carrier. *Journal of the American Chemical Society*, **2021**, 143, 223-231	16.4	20
149	Effects of hydrogen clusters on interface facilitated plasticity at semi-coherent bimetal interfaces. *Scripta Materialia*, **2021**, 190, 63-68	5.6	1
148	Two-Dimensional Carbonitride MXenes as an Efficient Electrocatalyst for Hydrogen Evolution. *Journal of Physical Chemistry C*, **2021**, 125, 4477-4488	3.8	3
147	Rational Design of Highly Stable and Active MXene-Based Bifunctional ORR/OER Double-Atom Catalysts. *Advanced Materials*, **2021**, 33, e2102595	24	27

146	Synergistic effect of solute and strain on the electrochemical degradation in representative Zn-based and Mg-based alloys. *Corrosion Science*, **2021**, 188, 109539	6.8	1
145	Synergistic Effect of Atomically Dispersed Ni-Zn Pair Sites for Enhanced CO Electroreduction. *Advanced Materials*, **2021**, 33, e2102212	24	33
144	Synergistic effect in ultrafine PtNiP nanowires for highly efficient electrochemical hydrogen evolution in alkaline electrolyte. *Applied Catalysis B: Environmental*, **2021**, 301, 120754	21.8	12
143	Insights into the Enhanced Structural and Thermal Stabilities of Nb-Substituted Lithium-Rich Layered Oxide Cathodes. *ACS Applied Materials & Interfaces*, **2021**, 13, 45619-45629	9.5	3
142	EAPOTs: An integrated empirical interatomic potential optimization platform for single elemental solids. *Computational Materials Science*, **2021**, 197, 110626	3.2	2
141	Mechanistic insights into interface-facilitated dislocation nucleation and phase transformation at semicoherent bimetal interfaces. *International Journal of Plasticity*, **2021**, 146, 103105	7.6	1
140	Magnetocrystalline anisotropy regulations in bulk L10-MnGa alloys by tailoring the tetragonal lattice parameter c: Selectively alloying Al and C atoms. *Journal of Alloys and Compounds*, **2021**, 881, 160646	5.7	2
139	Electrochemical Pourbaix diagrams of Mg-Zn alloys from first-principles calculations and experimental thermodynamic data. *Physical Chemistry Chemical Physics*, **2021**, 23, 19602-19610	3.6	1
138	Single-atom-Ni-decorated, nitrogen-doped carbon layers for efficient electrocatalytic CO2 reduction reaction. *Electrochemistry Communications*, **2020**, 116, 106758	5.1	13
137	Effects of solutes on dislocation nucleation and interface sliding of bimetal semi-coherent interface. *International Journal of Plasticity*, **2020**, 131, 102725	7.6	11
136	Interface facilitated transformation of voids directly into stacking fault tetrahedra. *Acta Materialia*, **2020**, 188, 623-634	8.4	9
135	Suppressed phase transition of a Rb/K incorporated inorganic perovskite with a water-repelling surface. *Nanoscale*, **2020**, 12, 6571-6581	7.7	7
134	Plastic flow between nanometer-spaced planar defects in nanostructured diamond and boron nitride. *Physical Review B*, **2020**, 101,	3.3	3
133	Modulating superexchange strength to achieve robust ferromagnetic couplings in two-dimensional semiconductors. *Physical Review B*, **2020**, 101,	3.3	3
132	Achieving high structure and voltage stability in cobalt-free Li-rich layered oxide cathodes via selective dual-cation doping. *Energy Storage Materials*, **2020**, 32, 37-45	19.4	30
131	Influence of high stacking-fault energy on the dissociation mechanisms of misfit dislocations at semi-coherent interfaces. *International Journal of Plasticity*, **2020**, 126, 102610	7.6	6
130	Mechanistic understanding of the size effect on shock facilitated dislocation nucleation at semicoherent interfaces. *Scripta Materialia*, **2020**, 178, 457-462	5.6	7
129	Ultrastrong □Bonded Interface as Ductile Plastic Flow Channel in Nanostructured Diamond. *ACS Applied Materials & Interfaces*, **2020**, 12, 4135-4142	9.5	5

128	Shearing dominated by the coupling of the interfacial misfit and atomic bonding at the FCC (111) semi-coherent interfaces. *Materials and Design*, **2020**, 186, 108294	8.1	4
127	Designing ultrahard nanostructured diamond through internal defects and interface engineering at different length scales. *Carbon*, **2020**, 170, 394-402	10.4	7
126	AADIS: An atomistic analyzer for dislocation character and distribution. *Computer Physics Communications*, **2020**, 247, 106857	4.2	10
125	Tunable magnetic order in transition metal doped, layered, and anisotropic Bi2O2Se: Competition between exchange interaction mechanisms. *Physical Review B*, **2019**, 100,	3.3	4
124	Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. *Acta Materialia*, **2019**, 181, 423-438	8.4	11
123	Uniaxial magnetocrystalline anisotropy of tetragonal Mn Ga100□(50 □x □75) alloys. *Journal of Magnetism and Magnetic Materials*, **2019**, 489, 165308	2.8	6
122	PNADIS: An automated Peierls□Nabarro analyzer for dislocation core structure and slip resistance. *Computer Physics Communications*, **2019**, 240, 60-73	4.2	10
121	Rational design of graphitic-inorganic Bi-layer artificial SEI for stable lithium metal anode. *Energy Storage Materials*, **2019**, 16, 426-433	19.4	64
120	Designing Flexible Quantum Spin Hall Insulators through 2D Ordered Hybrid Transition-Metal Carbides. *Journal of Physical Chemistry C*, **2019**, 123, 20664-20674	3.8	2
119	High-performance microwave absorption of hierarchical graphene-based and MWCNT-based full-carbon nanostructures. *Applied Surface Science*, **2019**, 493, 541-550	6.7	13
118	Designing ultrastrong 5d transition metal diborides with excellent stability for harsh service environments. *Physical Chemistry Chemical Physics*, **2019**, 21, 16095-16107	3.6	4
117	First-principles design of strong solids: Approaches and applications. *Physics Reports*, **2019**, 826, 1-49	27.7	17
116	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. *Chemical Reviews*, **2019**, 119, 11980-12031	68.1	137
115	Anchoring effect of distorted octahedra on the stability and strength of platinum metal pernitrides. *Physical Review Materials*, **2019**, 3,	3.2	1
114	A generalized solid strengthening rule for biocompatible Zn-based alloys, a comparison with Mg-based alloys. *Physical Chemistry Chemical Physics*, **2019**, 21, 22629-22638	3.6	1
113	ADAIS: Automatic Derivation of Anisotropic Ideal Strength via high-throughput first-principles computations. *Computer Physics Communications*, **2019**, 238, 244-253	4.2	11
112	Stronger and more failure-resistant with three-dimensional serrated bimetal interfaces. *Acta Materialia*, **2019**, 166, 231-245	8.4	22
111	Atomistic insight into the dislocation nucleation at crystalline/crystalline and crystalline/amorphous interfaces without full symmetry. *Acta Materialia*, **2019**, 162, 255-267	8.4	14

110	Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition-Metal Carbides. *Journal of Physical Chemistry C*, **2018**, 122, 4710-4722	3.8	22
109	Phonon-mediated stabilization and softening of 2D transition metal carbides: case studies of TiCO and MoCO. *Physical Chemistry Chemical Physics*, **2018**, 20, 14608-14618	3.6	6
108	High-throughput theoretical optimization of the hydrogen evolution reaction on MXenes by transition metal modification. *Journal of Materials Chemistry A*, **2018**, 6, 4271-4278	13	140
107	Stabilization of □phase in carbon-doped MnAl magnetic alloys. *Journal of Alloys and Compounds*, **2018**, 755, 257-264	5.7	26
106	Effect of dynamic evolution of misfit dislocation pattern on dislocation nucleation and shear sliding at semi-coherent bimetal interfaces. *Acta Materialia*, **2018**, 143, 107-120	8.4	32
105	AACSD: An atomistic analyzer for crystal structure and defects. *Computer Physics Communications*, **2018**, 222, 229-239	4.2	18
104	First-principles study on the electrical and thermal properties of the semiconducting Sc(CN)F MXene.. *RSC Advances*, **2018**, 8, 22452-22459	3.7	14
103	Highly Air-Stable Carbon-Based □CsPbI3 Perovskite Solar Cells with a Broadened Optical Spectrum. *ACS Energy Letters*, **2018**, 3, 1824-1831	20.1	183
102	High-throughput screening for superhard carbon and boron nitride allotropes with superior stiffness and strength. *Carbon*, **2018**, 137, 156-164	10.4	15
101	Unprecedented plastic flow channel in **B**28 through ultrasoft bonds: A challenge to superhardness. *Physical Review Materials*, **2018**, 2,	3.2	8
100	A synergetic stabilization and strengthening strategy for two-dimensional ordered hybrid transition metal carbides. *Physical Chemistry Chemical Physics*, **2018**, 20, 29684-29692	3.6	7
99	Magnetic origin of phase stability in cubic □MoN. *Applied Physics Letters*, **2018**, 113, 221901	3.4	6
98	Surface Electrochemical Stability and Strain-Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. *Advanced Functional Materials*, **2018**, 28, 1804867	15.6	21
97	Theoretical Investigation of 2D Layered Materials as Protective Films for Lithium and Sodium Metal Anodes. *Advanced Energy Materials*, **2017**, 7, 1602528	21.8	145
96	Theoretical investigations on helium trapping in the Zr/Ti2AlC interface. *Surface and Coatings Technology*, **2017**, 322, 19-24	4.4	14
95	New understanding of nano-scale interstitial dislocation loops in BCC iron. *Journal of Physics Condensed Matter*, **2017**, 29, 455301	1.8	11
94	An informatics guided classification of miscible and immiscible binary alloy systems. *Scientific Reports*, **2017**, 7, 9577	4.9	15
93	AELAS: Automatic ELAStic property derivations via high-throughput first-principles computation. *Computer Physics Communications*, **2017**, 220, 403-416	4.2	51

92	Designing flexible 2D transition metal carbides with strain-controllable lithium storage. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E11082-E11091	11.5	36
91	First-principles investigation of strain effects on the stacking fault energies, dislocation core structure, and Peierls stress of magnesium and its alloys. *Physical Review B*, **2017**, 95,	3.3	26
90	Ultrastrong Boron Frameworks in ZrB : A Highway for Electron Conducting. *Advanced Materials*, **2017**, 29, 1604003	24	50
89	Stacking stability and sliding mechanism in weakly bonded 2D transition metal carbides by van der Waals force. *RSC Advances*, **2017**, 7, 55912-55919	3.7	29
88	Miedema Calculator: A thermodynamic platform for predicting formation enthalpies of alloys within framework of Miedema Theory. *Computer Physics Communications*, **2016**, 209, 58-69	4.2	58
87	Domain-dependent electronic structure and optical absorption property in hybrid organic-inorganic perovskite. *Physical Chemistry Chemical Physics*, **2016**, 18, 27358-27365	3.6	9
86	Tuning lattice stability and mechanical strength of ultraincompressible tungsten carbides by varying the stacking sequence. *Physical Review B*, **2016**, 93,	3.3	12
85	Pinning effect of reactive elements on adhesion energy and adhesive strength of incoherent Al2O3/NiAl interface. *Physical Chemistry Chemical Physics*, **2016**, 18, 22864-73	3.6	12
84	Anomalous mechanical strengths and shear deformation paths of Al2O3 polymorphs with high ionicity. *RSC Advances*, **2016**, 6, 12885-12892	3.7	6
83	Crystal Field Splitting is Limiting the Stability and Strength of Ultra-incompressible Orthorhombic Transition Metal Tetraborides. *Scientific Reports*, **2016**, 6, 23088	4.9	17
82	Cooperative dissociations of misfit dislocations at bimetal interfaces. *APL Materials*, **2016**, 4, 111101	5.7	16
81	Structure and energetics of nanotwins in cubic boron nitrides. *Applied Physics Letters*, **2016**, 109, 081901	3.4	17
80	Manipulating dislocation nucleation and shear resistance of bimetal interfaces by atomic steps. *Acta Materialia*, **2016**, 113, 194-205	8.4	37
79	Stabilization and strengthening effects of functional groups in two-dimensional titanium carbide. *Physical Review B*, **2016**, 94,	3.3	103
78	Understanding the Anchoring Effect of Two-Dimensional Layered Materials for Lithium-Sulfur Batteries. *Nano Letters*, **2015**, 15, 3780-6	11.5	636
77	Mechanical strength and electronic instabilities in ultra-incompressible platinum dinitrides. *Physical Review B*, **2015**, 92,	3.3	15
76	Mapping Chemical Selection Pathways for Designing Multicomponent Alloys: an informatics framework for materials design. *Scientific Reports*, **2015**, 5, 17960	4.9	20
75	High Pressure Phase-Transformation Induced Texture Evolution and Strengthening in Zirconium Metal: Experiment and Modeling. *Scientific Reports*, **2015**, 5, 12552	4.9	18

74	Hardness, elastic, and electronic properties of chromium monoboride. *Applied Physics Letters*, **2015**, 106, 221902	3.4	46
73	Layer size effect on the shock compression behavior of fcc–bcc nanolaminates. *Acta Materialia*, **2014**, 79, 74-83	8.4	43
72	Statistically based assessment of formation enthalpy for intermetallic compounds. *Chemical Physics Letters*, **2014**, 612, 177-181	2.5	22
71	Bond deformation paths and electronic instabilities of ultraincompressible transition metal diborides: Case study of OsB2 and IrB2. *Physical Review B*, **2014**, 90,	3.3	19
70	The core structure of dislocations and their relationship to the material surface. *Journal of Applied Physics*, **2014**, 115, 134314	2.5	45
69	Interface dislocation patterns and dislocation nucleation in face-centered-cubic and body-centered-cubic bicrystal interfaces. *International Journal of Plasticity*, **2014**, 53, 40-55	7.6	93
68	Thermal stability of Cu–Nb nanolamellar composites fabricated via accumulative roll bonding. *Philosophical Magazine*, **2013**, 93, 718-735	1.6	75
67	Decomposition mechanism of Al1−xSixNy solid solution and possible mechanism of the formation of covalent nanocrystalline AlN/Si3N4 nanocomposites. *Acta Materialia*, **2013**, 61, 4226-4236	8.4	18
66	Dependence of equilibrium stacking fault width in fcc metals on the surface. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 025015	2	38
65	Mapping dislocation nucleation behavior from bimetal interfaces. *Acta Materialia*, **2013**, 61, 7488-7499	8.4	79
64	Origin of different plastic resistance of transition metal nitrides and carbides: Stiffer yet softer. *Scripta Materialia*, **2013**, 68, 913-916	5.6	19
63	Role of interface structure on the plastic response of Cu/Nb nanolaminates under shock compression: Non-equilibrium molecular dynamics simulations. *Scripta Materialia*, **2013**, 68, 114-117	5.6	70
62	Characterizing interface dislocations by atomically informed Frank-Bilby theory. *Journal of Materials Research*, **2013**, 28, 1646-1657	2.5	59
61	Interface-dependent nucleation in nanostructured layered composites. *APL Materials*, **2013**, 1, 032112	5.7	39
60	Structure–Property–Functionality of Bimetal Interfaces. *Jom*, **2012**, 64, 1192-1207	2.1	110
59	Atomic-scale study of nucleation of dislocations from fcc–bcc interfaces. *Acta Materialia*, **2012**, 60, 2855-2865	4.5	106
58	Structure and Property of Interfaces in ARB Cu/Nb Laminated Composites. *Jom*, **2012**, 64, 1208-1217	2.1	52
57	Synthesis, Crystal Structure, and Elastic Properties of Novel Tungsten Nitrides. *Chemistry of Materials*, **2012**, 24, 3023-3028	9.6	127

56	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites **2012**,		5
55	Experimental invalidation of phase-transition-induced elastic softening in CrN. *Physical Review B*, **2012**, 86,	3.3	42
54	Stability and strength of transition-metal tetraborides and triborides. *Physical Review Letters*, **2012**, 108, 255502	7.4	124
53	Superhard materials with low elastic moduli: Three-dimensional covalent bonding as the origin of superhardness in B6O. *Physical Review B*, **2011**, 83,	3.3	50
52	Dislocation nucleation mechanisms from fcc/bcc incoherent interfaces. *Scripta Materialia*, **2011**, 65, 1022-1025	3.6	102
51	Mechanical properties and hardness of boron and boron-rich solids. *Journal of Superhard Materials*, **2011**, 33, 409-420	0.9	41
50	Twinning in bcc metals under shock loading: a challenge to empirical potentials. *Philosophical Magazine Letters*, **2011**, 91, 731-740	1	50
49	Anisotropic ideal strengths of superhard monoclinic and tetragonal carbon and their electronic origin. *Physical Review B*, **2011**, 83,	3.3	29
48	Phase stabilities and decomposition mechanism in the ZrSiN system studied by combined ab initio DFT and thermodynamic calculation. *Acta Materialia*, **2011**, 59, 297-307	8.4	35
47	Study of spinodal decomposition and formation of nc-Al2O3/ZrO2 nanocomposites by combined ab initio density functional theory and thermodynamic modeling. *Acta Materialia*, **2011**, 59, 3498-3509	8.4	34
46	Thermodynamic stability and unusual strength of ultra-incompressible rhenium nitrides. *Physical Review B*, **2011**, 83,	3.3	48
45	Search for Ultrahard Materials and Recent Progress in the Understanding of Hardness Enhancement and Properties of Nanocomposites. *Solid State Phenomena*, **2010**, 159, 1-10	0.4	2
44	Shear-induced structural transformation and plasticity in ultraincompressible ReB2 limit its hardness. *Physical Review B*, **2010**, 82,	3.3	49
43	Design of ultrahard materials: Go nano!. *Philosophical Magazine*, **2010**, 90, 4101-4115	1.6	22
42	Understanding why the thinnest SiNx interface in transition-metal nitrides is stronger than the ideal bulk crystal. *Physical Review B*, **2010**, 81,	3.3	36
41	Superhard nanocomposites: Origin of hardness enhancement, properties and applications. *Surface and Coatings Technology*, **2010**, 204, 1898-1906	4.4	116
40	The Fundamentals of Hard and Superhard Nanocomposites and Heterostructures **2010**, 1-34		
39	The Fundamentals of Hard and Superhard Nanocomposites and Heterostructures **2010**, 1-34		

38	Electronic structure, stability, and mechanism of the decohesion and shear of interfaces in superhard nanocomposites and heterostructures. *Physical Review B*, **2009**, 79,	3.3	61
37	On the anisotropic shear resistance of hard transition metal nitrides TMN (TM=Ti, Zr, Hf). *Applied Physics Letters*, **2009**, 94, 121903	3.4	23
36	Effect of nanometer-sized grains on the superhardness of c-BC5: A first-principles study. *Physical Review B*, **2009**, 80,	3.3	17
35	Friedel oscillations are limiting the strength of superhard nanocomposites and heterostructures. *Physical Review Letters*, **2009**, 102, 015503	7.4	71
34	Deformation paths and atomistic mechanism of B4-B1 phase transformation in aluminium nitride. *Acta Materialia*, **2009**, 57, 2259-2265	8.4	22
33	Quadrotor aircraft control without velocity measurements **2009**,		18
32	Phase stabilities and thermal decomposition in the Zr1−xAlxN system studied by ab initio calculation and thermodynamic modeling. *Acta Materialia*, **2008**, 56, 968-976	8.4	69
31	Stability of TiBN solid solutions and the formation of nc-TiN/a-BN nanocomposites studied by combined ab initio and thermodynamic calculations. *Acta Materialia*, **2008**, 56, 4440-4449	8.4	38
30	Phase stabilities of self-organized nc-TiN/a-Si3N4 nanocomposites and of Ti1−xSixNy solid solutions studied by ab initio calculation and thermodynamic modeling. *Thin Solid Films*, **2008**, 516, 2264-2275	2.2	65
29	Anisotropic ideal strengths and chemical bonding of wurtzite BN in comparison to zincblende BN. *Physical Review B*, **2008**, 77,	3.3	76
28	Predicting the formation enthalpies of binary intermetallic compounds. *Chemical Physics Letters*, **2007**, 442, 511-514	2.5	62
27	Phase stabilities and spinodal decomposition in the Cr1−xAlxN system studied by ab initio LDA and thermodynamic modeling: Comparison with the Ti1−xAlxN and TiN/Si3N4 systems. *Acta Materialia*, **2007**, 55, 4615-4624	8.4	71
26	Metastable phases and spinodal decomposition in Ti1−xAlxN system studied by ab initio and thermodynamic modeling, a comparison with the TiN/Si3N4 system. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2007**, 448, 111-119	5.3	86
25	Chemistry, physics and fracture mechanics in search for superhard materials, and the origin of superhardness in nc-TiN/a-Si3N4 and related nanocomposites. *Journal of Physics and Chemistry of Solids*, **2007**, 68, 1161-1168	3.9	24
24	Mechanism of the B3 to B1 transformation in cubic AlN under uniaxial stress. *Physical Review B*, **2007**, 76,	3.3	23
23	Mechanical strengths of silicon nitrides studied by ab initio calculations. *Applied Physics Letters*, **2007**, 90, 191903	3.4	52
22	First principles studies of ideal strength and bonding nature of AlN polymorphs in comparison to TiN. *Applied Physics Letters*, **2007**, 91, 031906	3.4	62
21	Mechanical and electronic properties of hard rhenium diboride of low elastic compressibility studied by first-principles calculation. *Applied Physics Letters*, **2007**, 91, 201914	3.4	83

20	Crystalline-to-amorphous transition in Ti1−xSixN solid solution and the stability of fcc SiN studied by combined ab initio density functional theory and thermodynamic calculations. *Physical Review B*, **2007**, 76,	3.3	22
19	Origin of the hardness enhancement in superhard nc-TiN/a-Si3N4 and ultrahard nc-TiN/a-Si3N4/TiSi2 nanocomposites. *Philosophical Magazine Letters*, **2007**, 87, 955-966	1	58
18	On the spinodal nature of the phase segregation and formation of stable nanostructure in the TiSiN system. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2006**, 424, 128-137	5.3	85
17	Formation of amorphous alloys by ion beam mixing and its multiscale theoretical modeling in the equilibrium immiscible Sc-W system. *Journal of Physical Chemistry B*, **2005**, 109, 4391-7	3.4	13
16	Dual-Phase Metallic Glass and its Two-Dimensional Fractal Morphology. *Journal of the Physical Society of Japan*, **2005**, 74, 2937-2940	1.5	3
15	Thermodynamic criterion for the formation of Laves phases in binary transition-metal systems. *Philosophical Magazine Letters*, **2005**, 85, 283-287	1	14
14	Construction of n-body potentials for hcp-bcc metal systems within the framework of embedded atom method. *Physical Review B*, **2005**, 71,	3.3	9
13	Response to Comment on Proposed model for calculating the standard formation enthalpy of binary transition-metal systems [Appl. Phys. Lett. 86, 216103 (2005)]. *Applied Physics Letters*, **2005**, 86, 216104	3.4	2
12	Comment on Proposed model for calculating the standard formation enthalpy of binary transition-metal systems [Appl. Phys. Lett. 81, 1219 (2002)]. *Applied Physics Letters*, **2005**, 86, 216103	3.4	4
11	Comparative study of metastable phase formation in the immiscible CuW system byab initiocalculation andn-body potential. *Journal of Physics Condensed Matter*, **2004**, 16, 5251-5258	1.8	14
10	Proposed Calculation Method for Structural Formation Enthalpy including Magnetic Energy for Transition Metal Alloys. *Journal of the Physical Society of Japan*, **2004**, 73, 1097-1100	1.5	3
9	Study of metastable alloy formation by thermodynamic calculation and ion beam manipulation in an equilibrium immiscible AuW system. *Journal of Alloys and Compounds*, **2004**, 375, 179-185	5.7	2
8	Atomistic Modeling of Metastable Phase Selection of a Highly Immiscible AgW System. *Journal of the Physical Society of Japan*, **2004**, 73, 2023-2027	1.5	6
7	Metastable Phase Formed in Immiscible CuW Multilayers by Ion Mixing. *Japanese Journal of Applied Physics*, **2003**, 42, 7009-7012	1.4	14
6	Amorphous alloys synthesized by interface-assisted ion beam mixing in the AgW system with the largest positive heat of formation. *Journal of Materials Research*, **2003**, 18, 1499-1501	2.5	13
5	Ion Beam Manipulation to Fabricate Ordered Layered Structures and Amorphous Alloys in Some highly Immiscible Binary Metal Systems. *Materials Research Society Symposia Proceedings*, **2003**, 792, 499		
4	Magnetic properties of Co and Co-Ag alloys in equilibrium/nonequilibrium structures studied by ab initio calculations. *Physical Review B*, **2003**, 68,	3.3	24
3	Proposed model for calculating the standard formation enthalpy of binary transition-metal systems. *Applied Physics Letters*, **2002**, 81, 1219-1221	3.4	57

2	Comparative study of nonequilibrium phase of A3B and AB3 types in the NiMo system by first principles and thermodynamic calculations. *Journal of Materials Research*, **2002**, 17, 2720-2726	2.5	2
1	Single Atom-Modified Hybrid Transition Metal Carbides as Efficient Hydrogen Evolution Reaction Catalysts. *Advanced Functional Materials*,2104285	15.6	9