Shun-Li Shang

List of Publications by Year
in descending order

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257	9,574	36203	56606
papers	citations	51 h-index	83 g-index

265	265	265	8630
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles thermodynamics from phonon and Debye model: Application to Ni and Ni3Al. Computational Materials Science, 2010, 47, 1040-1048.	1.4	357
2	First-principles calculations of pure elements: Equations of state and elastic stiffness constants. Computational Materials Science, 2010, 48, 813-826.	1.4	259
3	First-principles elastic constants of Î±- and Î¸-Al2O3. Applied Physics Letters, 2007, 90, 101909.	1.5	238
4	Elastic constants of binary Mg compounds from first-principles calculations. Intermetallics, 2009, 17, 313-318.	1.8	212
5	Generalized stacking fault energy, ideal strength and twinnability of dilute Mg-based alloys: A first-principles study of shear deformation. Acta Materialia, 2014, 67, 168-180.	3.8	193
6	Effect of alloying elements on the elastic properties of Mg from first-principles calculations. Acta Materialia, 2009, 57, 3876-3884.	3.8	177
7	Diffusion coefficients of alloying elements in dilute Mg alloys: A comprehensive first-principles study. Acta Materialia, 2016, 103, 573-586.	3.8	169
8	A mixed-space approach to first-principles calculations of phonon frequencies for polar materials. Journal of Physics Condensed Matter, 2010, 22, 202201.	0.7	167
9	A first-principles approach to finite temperature elastic constants. Journal of Physics Condensed Matter, 2010, 22, 225404.	0.7	164
10	Exceptionally High Ionic Conductivity in Na₃P_{0.62}As_{0.38}S₄ with Improved Moisture Stability for Solidâ€State Sodiumâ€Ion Batteries. Advanced Materials, 2017, 29, 1605561.	11.1	164
11	Enthalpies of formation of magnesium compounds from first-principles calculations. Intermetallics, 2009, 17, 878-885.	1.8	159
12	A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields. Nature Nanotechnology, 2019, 14, 131-136.	15.6	150
13	Adsorption-controlled growth of La-doped BaSnO3 by molecular-beam epitaxy. APL Materials, 2017, 5, .	2.2	131
14	High Performance Anion Exchange Membrane Fuel Cells Enabled by Fluoropoly(olefin) Membranes. Advanced Functional Materials, 2019, 29, 1902059.	7.8	128
15	Structural and elastic properties of cubic and hexagonal TiN and AlN from first-principles calculations. Computational Materials Science, 2010, 48, 705-709.	1.4	126
16	First-principles calculations of lattice dynamics and thermal properties of polar solids. Npj Computational Materials, 2016, 2, .	3.5	119
17	A comprehensive first-principles study of pure elements: Vacancy formation and migration energies and self-diffusion coefficients. Acta Materialia, 2016, 109, 128-141.	3.8	117
18	Elastic properties of cubic and rhombohedral<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BiFeO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m first-principles calculations. Physical Review B, 2009, 80, .	1.1	116

#	Article	IF	Citations
19	Atomic structure of Zr41.2Ti13.8Cu12.5Ni10Be22.5 bulk metallic glass alloy. Acta Materialia, 2009, 57, 376-391.	3.8	108
20	Reassessment of the Alâ€“Mn system and a thermodynamic description of the Alâ€“Mgâ€“Mn system. International Journal of Materials Research, 2007, 98, 855-871.	0.1	106
21	First-principles calculations of the elastic, phonon and thermodynamic properties of Al12Mg17. Acta Materialia, 2010, 58, 4012-4018.	3.8	103
22	Effects of alloying element and temperature on the stacking fault energies of dilute Ni-base superalloys. Journal of Physics Condensed Matter, 2012, 24, 505403.	0.7	103
23	Lateral Versus Vertical Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides: Thermodynamic Insight into MoS₂. Nano Letters, 2016, 16, 5742-5750.	4.5	102
24	Effects of Alloying Elements on Stacking Fault Energies and Electronic Structures of Binary Mg Alloys: A First-Principles Study. Materials Research Letters, 2014, 2, 29-36.	4.1	95
25	Density-functional study of the thermodynamic properties and the pressureâ€“temperature phase diagram of Ti. Physical Review B, 2009, 80, .	1.1	94
26	Lattice dynamics, thermodynamics, and bonding strength of lithium-ion battery materials LiMPO₄(M = Mn, Fe, Co, and Ni): a comparative first-principles study. Journal of Materials Chemistry, 2012, 22, 1142-1149.	6.7	87
27	Effects of alloying elements on elastic properties of Ni3Al by first-principles calculations. Intermetallics, 2010, 18, 1163-1171.	1.8	86
28	Elastic properties of cubic, tetragonal and monoclinic ZrO2 from first-principles calculations. Journal of Nuclear Materials, 2011, 415, 13-17.	1.3	82
29	Extreme elastic anisotropy of cementite, Fe3C: First-principles calculations and experimental evidence. Scripta Materialia, 2008, 59, 814-817.	2.6	81
30	First-principles calculations of binary Al compounds: Enthalpies of formation and elastic properties. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 562-573.	0.7	81
31	Elastic anisotropy of Î³â€²-Fe4N and elastic grain interaction in Î³â€²-Fe4N1âˆ’y layers on Îµ-Fe: First-principles calculations and diffraction stress measurements. Acta Materialia, 2007, 55, 5833-5843.	3.8	78
32	Effects of alloying elements on elastic properties of Ni by first-principles calculations. Computational Materials Science, 2009, 47, 254-260.	1.4	78
33	First-principles calculations of phonon and thermodynamic properties in the boron-alkaline earth metal binary systems: B-Ca, B-Sr, and B-Ba. Physical Review B, 2007, 75, .	1.1	72
34	Temperature-dependent elastic stiffness constants of Îµ- and Îº-Al₂O₃from first-principles calculations. Journal of Physics Condensed Matter, 2010, 22, 375403.	0.7	70
35	The development and application of a thermodynamic database for magnesium alloys. Jom, 2008, 60, 45-47.	0.9	68
36	Fabrication and Characterization of Beaded SiC Quantum Rings with Anomalous Red Spectral Shift. Advanced Materials, 2012, 24, 5598-5603.	11.1	65

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37	Phase stability inÎ±- andÎ²-rhombohedral boron. Physical Review B, 2007, 75, .	1.1	64
38	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. Acta Materialia, 2012, 60, 5204-5216.	3.8	64
39	Thermodynamic and mechanical properties of lanthanumâ€“magnesium phases from density functional theory. Journal of Alloys and Compounds, 2012, 512, 296-310.	2.8	64
40	Temperature-dependent ideal strength and stacking fault energy of fcc Ni: a first-principles study of shear deformation. Journal of Physics Condensed Matter, 2012, 24, 155402.	0.7	64
41	Atomic and electronic basis for the serrations of refractory high-entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	64
42	Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study. Acta Materialia, 2015, 97, 75-85.	3.8	62
43	The structural evolution of boron carbide via ab initio calculations. Applied Physics Letters, 2007, 91, .	1.5	61
44	First-Principles Study of Lattice Dynamics and Thermodynamics of TiO2Polymorphs. Inorganic Chemistry, 2011, 50, 6996-7003.	1.9	61
45	Thermal Expansion Anomaly Regulated by Entropy. Scientific Reports, 2014, 4, 7043.	1.6	61
46	Synthesis science of SrRuO3 and CaRuO3 epitaxial films with high residual resistivity ratios. APL Materials, 2018, 6, .	2.2	61
47	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Domain Wall Energies and Structures: A Combined Experimental and Density Functional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mtext mathvariant="normal">Theory</mml:mtext><mml:mo mathvariant="bold">+</mml:mo><mml:mi mathvariant="bold">U</mml:mi></mml:math>Study. Physical Review Letters, 2013, 110, 267601.	2.9	59
48	Vacancy mechanism of oxygen diffusivity in bcc Fe: A first-principles study. Corrosion Science, 2014, 83, 94-102.	3.0	56
49	First-principles lattice dynamics and heat capacity of BiFeO3. Acta Materialia, 2011, 59, 4229-4234.	3.8	55
50	A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8. Nano Energy, 2018, 47, 325-330.	8.2	55
51	Computation of entropies and phase equilibria in refractory V-Nb-Mo-Ta-W high-entropy alloys. Acta Materialia, 2018, 143, 88-101.	3.8	55
52	Temperature dependent elastic coefficients of Mg2X (X=Si, Ge, Sn, Pb) compounds from first-principles calculations. Journal of Alloys and Compounds, 2010, 498, 191-198.	2.8	53
53	A combined cluster variation method and ab initio approach to the Î³-Fe[N]/Î³â€²-Fe4N1âˆ’x phase equilibrium. Acta Materialia, 2005, 53, 255-264.	3.8	51
54	Atomic control of active-site ensembles in ordered alloys to enhance hydrogenation selectivity. Nature Chemistry, 2022, 14, 523-529.	6.6	51

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55	al, vibrational, and thermodynamic properties of ordered and disordered Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mrow /></mml:mrow></mml:math>	1.1	49
56	A comprehensive first-principles study of solute elements in dilute Ni alloys: Diffusion coefficients and their implications to tailor creep rate. Acta Materialia, 2018, 157, 126-141.	3.8	49
57	First-principles lattice dynamics, thermodynamics, and elasticity of Cr2O3. Surface Science, 2012, 606, 1422-1425.	0.8	47
58	Reaction behavior and pore formation mechanism of TiAlâ€“Nb porous alloys prepared by elemental powder metallurgy. Intermetallics, 2014, 44, 1-7.	1.8	47
59	Origin of Outstanding Phase and Moisture Stability in a Na₃P_{1â€“x}As_xS₄ Superionic Conductor. ACS Applied Materials & Interfaces, 2017, 9, 16261-16269.	4.0	46
60	Local lattice distortion mediated formation of stacking faults in Mg alloys. Acta Materialia, 2019, 170, 231-239.	3.8	45
61	Thermodynamic fluctuations in magnetic states: Fe₃Pt as a prototype. Philosophical Magazine Letters, 2010, 90, 851-859.	0.5	44
62	Origin of negative thermal expansion phenomenon in solids. Scripta Materialia, 2011, 65, 664-667.	2.6	44
63	Martensitic transition in Fe via Bain path at finite temperatures: A comprehensive first-principles study. Acta Materialia, 2018, 147, 261-276.	3.8	44
64	Thermodynamic fluctuations between magnetic states from first-principles phonon calculations: The case of bcc Fe. Physical Review B, 2010, 82, .	1.1	42
65	Effects of alloying elements on thermal expansions of Î³-Ni and Î³â€²-Ni3Al by first-principles calculations. Acta Materialia, 2012, 60, 1846-1856.	3.8	42
66	Pore structure and gas permeability of high Nb-containing TiAl porous alloys by elemental powder metallurgy for microfiltration application. Intermetallics, 2013, 33, 2-7.	1.8	42
67	Electronic structures of long periodic stacking order structures in Mg: A first-principles study. Journal of Alloys and Compounds, 2014, 586, 656-662.	2.8	42
68	A novel hot pack rolling of high Nbâ€“TiAl sheet from cast ingot. Intermetallics, 2015, 67, 19-25.	1.8	42
69	Synthesis and understanding of Na11Sn2PSe12 with enhanced ionic conductivity for all-solid-state Na-ion battery. Energy Storage Materials, 2019, 17, 70-77.	9.5	42
70	Anomalous energy pathway of vacancy migration and self-diffusion in hcp Ti. Physical Review B, 2011, 83, .	1.1	41
71	First-principles calculations of phonon and thermodynamic properties of Fe-Si compounds. Intermetallics, 2011, 19, 1374-1384.	1.8	40
72	A first-principles study of self-diffusion coefficients of fcc Ni. Computational Materials Science, 2014, 86, 17-23.	1.4	40

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73	Ti-substituted Li[Li_{0.26}Mn_{0.6â˜'x}Ti_xNi_{0.07}Co_{0.07}]O₂ layered cathode material with improved structural stability and suppressed voltage fading. Journal of Materials Chemistry A, 2015, 3, 17376-17384.	5.2	40
74	Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L12 Co3(Al, TM): A comprehensive first-principles study. Acta Materialia, 2018, 145, 30-40.	3.8	40
75	A first-principles study of the diffusion coefficients of alloying elements in dilute Î±-Ti alloys. Physical Chemistry Chemical Physics, 2016, 18, 16870-16881.	1.3	39
76	Insight into Î³-Ni/Î³â€²-Ni3Al interfacial energy affected by alloying elements. Materials and Design, 2017, 133, 39-46.	3.3	39
77	Atomic structure and diffusivity in liquid Al80Ni20 by ab initio molecular dynamics simulations. Physica B: Condensed Matter, 2011, 406, 3089-3097.	1.3	38
78	Effects of alloying elements on the elastic properties of bcc Ti-X alloys from first-principles calculations. Computational Materials Science, 2018, 142, 215-226.	1.4	38
79	Adsorption-controlled growth of Ga2O3 by suboxide molecular-beam epitaxy. APL Materials, 2021, 9, .	2.2	38
80	Electron localization morphology of the stacking faults in Mg: A first-principles study. Chemical Physics Letters, 2012, 551, 121-125.	1.2	37
81	Mixed-space approach for calculation of vibration-induced dipole-dipole interactions. Physical Review B, 2012, 85, .	1.1	37
82	Nature of ferroelectric-paraelectric phase transition and origin of negative thermal expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>PbTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2015, 91, .	1.1	37
83	First-principles study of adsorption and diffusion of oxygen on surfaces of TiN, ZrN and HfN. Applied Surface Science, 2018, 452, 457-462.	3.1	37
84	A first-principles study of structure, elasticity and thermal decomposition of Ti1â˜'xTMxN alloys (TM=Y,) Tj ETQq0 0 0 rgBT /Overlock 10	2.2	36
85	Calculated strain energy of hexagonal epitaxial thin films. Journal of Crystal Growth, 2002, 240, 6-13.	0.7	35
86	Density-functional study of the pressure-induced phase transitions in Ti at zero Kelvin. Physical Review B, 2009, 79, .	1.1	34
87	Solvus boundaries of (meta)stable phases in the Alâ€"Mgâ€"Si system: First-principles phonon calculations and thermodynamic modeling. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 20-25.	0.7	34
88	Thermodynamics of the Sâ€"Sn system: Implication for synthesis of earth abundant photovoltaic absorber materials. Solar Energy, 2016, 125, 314-323.	2.9	34
89	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. Acta Materialia, 2021, 217, 117169.	3.8	34
90	Icosahedral ordering in Zr41Ti14Cu12.5Ni10Be22.5 bulk metallic glass. Applied Physics Letters, 2008, 92, 201913.	1.5	33

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91	A thermodynamic framework for a system with itinerant-electron magnetism. Journal of Physics Condensed Matter, 2009, 21, 326003.	0.7	33
92	First-principles studies on vacancy-modified interstitial diffusion mechanism of oxygen in nickel, associated with large-scale atomic simulation techniques. Journal of Applied Physics, 2014, 115, .	1.1	33
93	Insight into structural, elastic, phonon, and thermodynamic properties of Î±-sulfur and energy-related sulfides: a comprehensive first-principles study. Journal of Materials Chemistry A, 2015, 3, 8002-8014.	5.2	33
94	Effects of alloying elements and temperature on the elastic properties of W-based alloys by first-principles calculations. Journal of Alloys and Compounds, 2016, 671, 267-275.	2.8	33
95	First-principles study of the mechanical properties and phase stability of TiO2. Computational Materials Science, 2014, 83, 114-119.	1.4	32
96	Metastable trigonal SnP: A promising anode material for potassium-ion battery. Carbon, 2020, 168, 468-474.	5.4	32
97	Lattice dynamics and anomalous bonding in rhombohedral As: First-principles supercell method. Physical Review B, 2007, 76, .	1.1	31
98	Broken symmetry, strong correlation, and splitting between longitudinal and transverse optical phonons of MnO and NiO from first principles. Physical Review B, 2010, 82, .	1.1	31
99	Magnetic thermodynamics of fcc Ni from first-principles partition function approach. Journal of Applied Physics, 2010, 108, .	1.1	31
100	On the scaling factor in Debyeâ€“GrÃ¼neisen model: A case study of the Mgâ€“Zn binary system. Computational Materials Science, 2015, 98, 34-41.	1.4	31
101	Elastic knowledge base of bcc Ti alloys from first-principles calculations and CALPHAD-based modeling. Computational Materials Science, 2017, 140, 121-139.	1.4	30
102	Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. Acta Materialia, 2015, 82, 287-294.	3.8	29
103	Phase stability of the Cu-Sn-S system and optimal growth conditions for earth-abundant Cu2SnS3 solar materials. Solar Energy, 2017, 155, 745-757.	2.9	29
104	Accelerating exploitation of Co-Al-based superalloys from theoretical study. Materials and Design, 2018, 142, 139-148.	3.3	29
105	Microstructural characteristics and crack formation in additively manufactured bimetal material of 316L stainless steel and Inconel 625. Additive Manufacturing, 2020, 32, 101037.	1.7	29
106	Short-to-medium-range order in Mg65Cu25Y10 metallic glass. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 3078-3084.	0.9	28
107	Thermodynamic properties of Laves phases in the Mgâ€“Alâ€“Ca system at finite temperature from first-principles. Intermetallics, 2012, 22, 17-23.	1.8	28
108	Thermodynamic description of the Ti-Mo-Nb-Ta-Zr system and its implications for phase stability of Ti bio-implant materials. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 72-84.	0.7	28

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109	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Î±-Mg₃Sb₂. ACS Applied Energy Materials, 2018, 1, 6600-6608.	2.5	28
110	Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis. APL Materials, 2020, 8, .	2.2	28
111	Effects of pressure and vibration on the thermal decomposition of cubic Ti1-x Al x N, Ti1-x Zr x N, and Zr1-x Al x N coatings: a first-principles study. Journal of Materials Science, 2012, 47, 7621-7627.	1.7	26
112	Understanding slow-growing alumina scale mediated by reactive elements: Perspective via local metal-oxygen bonding strength. Scripta Materialia, 2018, 150, 139-142.	2.6	26
113	Thermodynamic modeling of fcc order/disorder transformations in the Coâ€“Pt system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 323-330.	0.7	25
114	Anisotropy and temperature dependence of structural, thermodynamic, and elastic properties of crystalline cellulose I_{Î²}: a first-principles investigation. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 085012.	0.8	25
115	First-principles thermodynamic theory of Seebeck coefficients. Physical Review B, 2018, 98, .	1.1	25
116	First-principles study of elastic and phonon properties of the heavy fermion compound CeMg. Journal of Physics Condensed Matter, 2009, 21, 246001.	0.7	24
117	Entropy favored ordering: Phase stability of Ni3Pt revisited by first-principles. Intermetallics, 2010, 18, 961-964.	1.8	24
118	Structural, phonon and thermodynamic properties of fcc-based metal nitrides from first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2012, 37, 126-131.	0.7	24
119	Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias. Advanced Materials, 2016, 28, 118-123.	11.1	24
120	Power law scaled hardness of Mn strengthened nanocrystalline Al Mn non-equilibrium solid solutions. Scripta Materialia, 2016, 120, 31-36.	2.6	24
121	C15 NbCr2 Laves phase with mechanical properties beyond Pughâ€™s criterion. Computational Materials Science, 2016, 121, 167-173.	1.4	24
122	Data set for diffusion coefficients and relative creep rate ratios of 26 dilute Ni-X alloy systems from first-principles calculations. Data in Brief, 2018, 20, 1537-1551.	0.5	24
123	Phonon and thermodynamic properties of Alâ€“Mn compounds: A first-principles study. Computational Materials Science, 2011, 50, 2096-2103.	1.4	23
124	Phonon dispersions in random alloys: a method based on special quasi-random structure force constants. Journal of Physics Condensed Matter, 2011, 23, 485403.	0.7	23
125	Accurate calculations of phonon dispersion in CaF<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 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>. Physical Review B, 2013, 88, .	1.1	23
126	Control of Phase in Tin Sulfide Thin Films Produced via RF-Sputtering of SnS2 Target with Post-deposition Annealing. Journal of Electronic Materials, 2016, 45, 499-508.	1.0	23

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127	Phase transformation in Tiâ€“48Alâ€“6Nb porous alloys and its influence on pore properties. Materials and Design, 2015, 83, 508-513.	3.3	22
128	First-principles investigation of phase stability, elastic and thermodynamic properties in L12 Co3(Al,Mo,Nb) phase. Intermetallics, 2016, 78, 1-7.	1.8	22
129	Elastic3rd: A tool for calculating third-order elastic constants from first-principles calculations. Computer Physics Communications, 2021, 261, 107777.	3.0	22
130	Hyperfine interactions in hexagonal Îµ-Fe6Ny phase investigated by MÃ¶ssbauer spectroscopy and ab initio calculations. Acta Materialia, 2006, 54, 2407-2417.	3.8	21
131	The influence of interstitial distribution on phase stability and properties of hexagonal Îµ-Fe6Cx, Îµ-Fe6Ny and Îµ-Fe6CxNy phases: A first-principles calculation. Acta Materialia, 2008, 56, 719-725.	3.8	21
132	Thermodynamic modeling of Mgâ€“Caâ€“Ce system by combining first-principles and CALPHAD method. Journal of Alloys and Compounds, 2008, 463, 294-301.	2.8	21
133	Crystal structure determination of HÃgg carbide, Ï‡-Fe₅C₂ by first-principles calculations and Rietveld refinement. Zeitschrift FÃ¼r Kristallographie, 2012, 227, 207-220.	1.1	21
134	Effects of Composition on Atomic Structure, Diffusivity, and Viscosity of Liquid Al-Zr Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 3471-3480.	1.1	21
135	Revealing the Microstates of Body-Centered-Cubic (BCC) Equiatomic High Entropy Alloys. Journal of Phase Equilibria and Diffusion, 2017, 38, 404-415.	0.5	21
136	Elastic properties of long periodic stacking ordered phases in Mg-Gd-Al alloys: A first-principles study. Intermetallics, 2018, 98, 18-27.	1.8	21
137	C-vacancy concentration in cementite, Fe3C1â^', in equilibrium with Î±-Fe[C] and Î³-Fe[C]. Acta Materialia, 2015, 86, 374-384.	3.8	20
138	Unveiling non-equilibrium metallurgical phases in dissimilar Al-Cu joints processed by vaporizing foil actuator welding. Materials and Design, 2020, 186, 108306.	3.3	20
139	Density Functional Theory-Based Database Development and CALPHAD Automation. Jom, 2013, 65, 1533-1539.	0.9	19
140	First-principles calculations and thermodynamic modeling of the Snâ^'Sr and Mgâ^'Snâ^'Sr systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 46, 237-248.	0.7	19
141	Effective elastic properties of polycrystals based on phase-field description. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 554, 67-71.	2.6	18
142	Cation Disorder Regulation by Microstate Configurational Entropy in Photovoltaic Absorber Materials Cu2ZnSn(S,Se)4. Journal of Physical Chemistry C, 2014, 118, 24884-24889.	1.5	18
143	Data set for diffusion coefficients of alloying elements in dilute Mg alloys from first-principles. Data in Brief, 2015, 5, 900-912.	0.5	18
144	Quantum behavior of water nano-confined in beryl. Journal of Chemical Physics, 2017, 146, 124307.	1.2	18

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145	Fundamentals of Thermal Expansion and Thermal Contraction. Materials, 2017, 10, 410.	1.3	18
146	Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. Acta Materialia, 2019, 181, 423-438.	3.8	18
147	Unveiling dislocation characteristics in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Al</mml:mi></mml:mrow></mml:math> from stacking fault energy and ideal strength: A first-principles study via pure alias shear deformation. Physical Review B, 2020, 101, .	1.1	18
148	Thermodynamic modelling of the Bâ€“Ca, Bâ€“Sr and Bâ€“Ba systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2007, 31, 286-291.	0.7	17
149	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.	0.7	17
150	Thermodynamic Properties of Co₃O₄and Sr₆Co₅O₁₅from First-Principles. Inorganic Chemistry, 2010, 49, 10291-10298.	1.9	17
151	Integrating computational modeling and first-principles calculations to predict stacking fault energy of dilute multicomponent Ni-base alloys. Computational Materials Science, 2014, 91, 50-55.	1.4	17
152	Solid-Solution Hardening in Mg-Gd-TM (TMÂ=ÂAg, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study. Jom, 2015, 67, 2433-2441.	0.9	17
153	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TMÂ=ÂCr, Ni, Ta and Zr) alloys. Materials Chemistry and Physics, 2015, 162, 748-756.	2.0	17
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