Shun-Li Shang

List of Publications by Citations

254	7,188	46	72
papers	citations	h-index	g-index
265	8,354	4.9	6.01
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
254	First-principles thermodynamics from phonon and Debye model: Application to Ni and Ni3Al. *Computational Materials Science*, **2010**, 47, 1040-1048	3.2	278
253	First-principles calculations of pure elements: Equations of state and elastic stiffness constants. *Computational Materials Science*, **2010**, 48, 813-826	3.2	219
252	First-principles elastic constants of □and □Al2O3. *Applied Physics Letters*, **2007**, 90, 101909	3.4	183
251	Elastic constants of binary Mg compounds from first-principles calculations. *Intermetallics*, **2009**, 17, 313-318	3.5	168
250	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	8.4	151
249	Effect of alloying elements on the elastic properties of Mg from first-principles calculations. *Acta Materialia*, **2009**, 57, 3876-3884	8.4	137
248	A first-principles approach to finite temperature elastic constants. *Journal of Physics Condensed Matter*, **2010**, 22, 225404	1.8	136
247	Enthalpies of formation of magnesium compounds from first-principles calculations. *Intermetallics*, **2009**, 17, 878-885	3.5	131
246	A mixed-space approach to first-principles calculations of phonon frequencies for polar materials. *Journal of Physics Condensed Matter*, **2010**, 22, 202201	1.8	129
245	Exceptionally High Ionic Conductivity in Na P As S with Improved Moisture Stability for Solid-State Sodium-Ion Batteries. *Advanced Materials*, **2017**, 29, 1605561	24	122
244	Diffusion coefficients of alloying elements in dilute Mg alloys: A comprehensive first-principles study. *Acta Materialia*, **2016**, 103, 573-586	8.4	108
243	Structural and elastic properties of cubic and hexagonal TiN and AlN from first-principles calculations. *Computational Materials Science*, **2010**, 48, 705-709	3.2	99
242	Adsorption-controlled growth of La-doped BaSnO3 by molecular-beam epitaxy. *APL Materials*, **2017**, 5, 116107	5.7	98
241	A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields. *Nature Nanotechnology*, **2019**, 14, 131-136	28.7	98
240	Elastic properties of cubic and rhombohedral BiFeO3 from first-principles calculations. *Physical Review B*, **2009**, 80,	3.3	97
239	Atomic structure of Zr41.2Ti13.8Cu12.5Ni10Be22.5 bulk metallic glass alloy. *Acta Materialia*, **2009**, 57, 376-391	8.4	93
238	Reassessment of the Al□Mn system and a thermodynamic description of the Al□Mg□Mn system. *International Journal of Materials Research*, **2007**, 98, 855-871	0.5	92

237	First-principles calculations of lattice dynamics and thermal properties of polar solids. *Npj Computational Materials*, **2016**, 2,	10.9	88
236	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	7.4	85
235	First-principles calculations of the elastic, phonon and thermodynamic properties of Al12Mg17. *Acta Materialia*, **2010**, 58, 4012-4018	8.4	81
234	Density-functional study of the thermodynamic properties and the pressure□emperature phase diagram of Ti. *Physical Review B*, **2009**, 80,	3.3	79
233	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		78
232	Effects of alloying element and temperature on the stacking fault energies of dilute Ni-base superalloys. *Journal of Physics Condensed Matter*, **2012**, 24, 505403	1.8	73
231	High Performance Anion Exchange Membrane Fuel Cells Enabled by Fluoropoly(olefin) Membranes. *Advanced Functional Materials*, **2019**, 29, 1902059	15.6	72
230	Extreme elastic anisotropy of cementite, Fe3C: First-principles calculations and experimental evidence. *Scripta Materialia*, **2008**, 59, 814-817	5.6	72
229	Effects of alloying elements on elastic properties of Ni3Al by first-principles calculations. *Intermetallics*, **2010**, 18, 1163-1171	3.5	71
228	Elastic anisotropy of □-Fe4N and elastic grain interaction in □-Fe4N1□ layers on □-Fe: First-principles calculations and diffraction stress measurements. *Acta Materialia*, **2007**, 55, 5833-5843	8.4	71
227	Lateral Versus Vertical Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides: Thermodynamic Insight into MoS2. *Nano Letters*, **2016**, 16, 5742-50	11.5	70
226	The development and application of a thermodynamic database for magnesium alloys. *Jom*, **2008**, 60, 45-47	2.1	67
225	A comprehensive first-principles study of pure elements: Vacancy formation and migration energies and self-diffusion coefficients. *Acta Materialia*, **2016**, 109, 128-141	8.4	66
224	Effects of alloying elements on elastic properties of Ni by first-principles calculations. *Computational Materials Science*, **2009**, 47, 254-260	3.2	66
223	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,	3.3	64
222	Elastic properties of cubic, tetragonal and monoclinic ZrO2 from first-principles calculations. *Journal of Nuclear Materials*, **2011**, 415, 13-17	3.3	61
221	Fabrication and characterization of beaded SiC quantum rings with anomalous red spectral shift. *Advanced Materials*, **2012**, 24, 5598-603	24	59
220	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. *Acta Materialia*, **2012**, 60, 5204-5216	8.4	58

219	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	1.9	57
218	First-principles study of lattice dynamics and thermodynamics of TiO2 polymorphs. *Inorganic Chemistry*, **2011**, 50, 6996-7003	5.1	57
217	Thermodynamic and mechanical properties of lanthanum□magnesium phases from density functional theory. *Journal of Alloys and Compounds*, **2012**, 512, 296-310	5.7	56
216	The structural evolution of boron carbide via ab initio calculations. *Applied Physics Letters*, **2007**, 91, 231915	3.4	56
215	Phase stability in □and □rhombohedral boron. *Physical Review B*, **2007**, 75,	3.3	55
214	Temperature-dependent elastic stiffness constants of □and □Al2O3 from first-principles calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 375403	1.8	54
213	BiFeO3 domain wall energies and structures: a combined experimental and density functional theory+U study. *Physical Review Letters*, **2013**, 110, 267601	7.4	49
212	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	1.8	49
211	Vacancy mechanism of oxygen diffusivity in bcc Fe: A first-principles study. *Corrosion Science*, **2014**, 83, 94-102	6.8	47
210	A combined cluster variation method and ab initio approach to the □Fe[N]/□-Fe4N1□ phase equilibrium. *Acta Materialia*, **2005**, 53, 255-264	8.4	47
209	Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study. *Acta Materialia*, **2015**, 97, 75-85	8.4	46
208	Thermal expansion anomaly regulated by entropy. *Scientific Reports*, **2014**, 4, 7043	4.9	46
207	First-principles lattice dynamics and heat capacity of BiFeO3. *Acta Materialia*, **2011**, 59, 4229-4234	8.4	46
206	A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8. *Nano Energy*, **2018**, 47, 325-330	17.1	45
205	First-principles lattice dynamics, thermodynamics, and elasticity of Cr2O3. *Surface Science*, **2012**, 606, 1422-1425	1.8	42
204	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	5.7	42
203	Structural, vibrational, and thermodynamic properties of ordered and disordered Ni1□Ptx alloys from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	42
202	Synthesis science of SrRuO3 and CaRuO3 epitaxial films with high residual resistivity ratios. *APL Materials*, **2018**, 6, 046101	5.7	41

201	Computation of entropies and phase equilibria in refractory V-Nb-Mo-Ta-W high-entropy alloys. *Acta Materialia*, **2018**, 143, 88-101	8.4	39
200	Atomic and electronic basis for the serrations of refractory high-entropy alloys. *Npj Computational Materials*, **2017**, 3,	10.9	39
199	Origin of Outstanding Phase and Moisture Stability in a NaPAsS Superionic Conductor. *ACS Applied Materials & Interfaces*, **2017**, 9, 16261-16269	9.5	38
198	Atomic structure and diffusivity in liquid Al80Ni20 by ab initio molecular dynamics simulations. *Physica B: Condensed Matter*, **2011**, 406, 3089-3097	2.8	37
197	Electronic structures of long periodic stacking order structures in Mg: A first-principles study. *Journal of Alloys and Compounds*, **2014**, 586, 656-662	5.7	34
196	Anomalous energy pathway of vacancy migration and self-diffusion in hcp Ti. *Physical Review B*, **2011**, 83,	3.3	34
195	Ti-substituted Li[Li0.26Mn0.6□TixNi0.07Co0.07]O2 layered cathode material with improved structural stability and suppressed voltage fading. *Journal of Materials Chemistry A*, **2015**, 3, 17376-17384	13	33
194	A novel hot pack rolling of high Nb□TiAl sheet from cast ingot. *Intermetallics*, **2015**, 67, 19-25	3.5	33
193	Mixed-space approach for calculation of vibration-induced dipole-dipole interactions. *Physical Review B*, **2012**, 85,	3.3	33
192	Thermodynamic fluctuations between magnetic states from first-principles phonon calculations: The case of bcc Fe. *Physical Review B*, **2010**, 82,	3.3	33
191	Reaction behavior and pore formation mechanism of TiAl□Nb porous alloys prepared by elemental powder metallurgy. *Intermetallics*, **2014**, 44, 1-7	3.5	32
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189	Origin of negative thermal expansion phenomenon in solids. *Scripta Materialia*, **2011**, 65, 664-667	5.6	32
188	Calculated strain energy of hexagonal epitaxial thin films. *Journal of Crystal Growth*, **2002**, 240, 6-13	1.6	32
187	First-principles calculations of phonon and thermodynamic properties of Fe-Si compounds. *Intermetallics*, **2011**, 19, 1374-1384	3.5	31
186	Density-functional study of the pressure-induced phase transitions in Ti at zero Kelvin. *Physical Review B*, **2009**, 79,	3.3	31
185	Icosahedral ordering in Zr41Ti14Cu12.5Ni10Be22.5 bulk metallic glass. *Applied Physics Letters*, **2008**, 92, 201913	3.4	31
184	Insight into structural, elastic, phonon, and thermodynamic properties of □sulfur and energy-related sulfides: a comprehensive first-principles study. *Journal of Materials Chemistry A*, **2015**, 3, 8002-8014	13	29

183	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, 043501	2.5	29
182	Electron localization morphology of the stacking faults in Mg: A first-principles study. *Chemical Physics Letters*, **2012**, 551, 121-125	2.5	29
181	Thermodynamic fluctuations in magnetic states: Fe3Pt as a prototype. *Philosophical Magazine Letters*, **2010**, 90, 851-859	1	29
180	Effects of alloying elements on thermal expansions of □Ni and □-Ni3Al by first-principles calculations. *Acta Materialia*, **2012**, 60, 1846-1856	8.4	28
179	Broken symmetry, strong correlation, and splitting between longitudinal and transverse optical phonons of MnO and NiO from first principles. *Physical Review B*, **2010**, 82,	3.3	28
178	Lattice dynamics and anomalous bonding in rhombohedral As: First-principles supercell method. *Physical Review B*, **2007**, 76,	3.3	28
177	A first-principles study of the diffusion coefficients of alloying elements in dilute □Ti alloys. *Physical Chemistry Chemical Physics*, **2016**, 18, 16870-81	3.6	28
176	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	8.4	28
175	On the scaling factor in Debye□Grüneisen model: A case study of the Mg□Zn binary system. *Computational Materials Science*, **2015**, 98, 34-41	3.2	27
174	Thermodynamics of the S□Sn system: Implication for synthesis of earth abundant photovoltaic absorber materials. *Solar Energy*, **2016**, 125, 314-323	6.8	27
173	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	8.4	27
172	A first-principles study of self-diffusion coefficients of fcc Ni. *Computational Materials Science*, **2014**, 86, 17-23	3.2	27
171	First-principles study of the mechanical properties and phase stability of TiO2. *Computational Materials Science*, **2014**, 83, 114-119	3.2	26
170	Synthesis and understanding of Na11Sn2PSe12 with enhanced ionic conductivity for all-solid-state Na-ion battery. *Energy Storage Materials*, **2019**, 17, 70-77	19.4	26
169	Phase stability of the Cu-Sn-S system and optimal growth conditions for earth-abundant Cu2SnS3 solar materials. *Solar Energy*, **2017**, 155, 745-757	6.8	25
168	Nature of ferroelectric-paraelectric phase transition and origin of negative thermal expansion in PbTiO3. *Physical Review B*, **2015**, 91,	3.3	25
167	Magnetic thermodynamics of fcc Ni from first-principles partition function approach. *Journal of Applied Physics*, **2010**, 108, 123514	2.5	25
166	A first-principles study of structure, elasticity and thermal decomposition of Ti1 □xTMxN alloys (TM = Y, Zr, Nb, Hf, and Ta). *Surface and Coatings Technology*, **2015**, 264, 41-48	4.4	24

165	Short-to-medium-range order in Mg65Cu25Y10 metallic glass. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 3078-3084	2.3	24
164	Local lattice distortion mediated formation of stacking faults in Mg alloys. *Acta Materialia*, **2019**, 170, 231-239	8.4	23
163	Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. *Acta Materialia*, **2015**, 82, 287-294	8.4	23
162	Thermodynamic properties of Laves phases in the MgAlCa system at finite temperature from first-principles. *Intermetallics*, **2012**, 22, 17-23	3.5	23
161	Entropy favored ordering: Phase stability of Ni3Pt revisited by first-principles. *Intermetallics*, **2010**, 18, 961-964	3.5	23
160	Solvus boundaries of (meta)stable phases in the AlMgSi system: First-principles phonon calculations and thermodynamic modeling. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2010**, 34, 20-25	1.9	23
159	A thermodynamic framework for a system with itinerant-electron magnetism. *Journal of Physics Condensed Matter*, **2009**, 21, 326003	1.8	23
158	Effects of alloying elements on the elastic properties of bcc Ti-X alloys from first-principles calculations. *Computational Materials Science*, **2018**, 142, 215-226	3.2	22
157	Insight into γ-Ni/γ′-Ni3Al interfacial energy affected by alloying elements. *Materials and Design*, **2017**, 133, 39-46	8.1	21
156	Accurate calculations of phonon dispersion in CaF2 and CeO2. *Physical Review B*, **2013**, 88,	3.3	21
155	Crystal structure determination of Hägg carbide, χ-Fe5C2 by first-principles calculations and Rietveld refinement. *Zeitschrift Für Kristallographie*, **2012**, 227, 207-220		21
154	First-principles study of elastic and phonon properties of the heavy fermion compound CeMg. *Journal of Physics Condensed Matter*, **2009**, 21, 246001	1.8	21
153	The influence of interstitial distribution on phase stability and properties of hexagonal ε-Fe6Cx, ε-Fe6Ny and ε-Fe6CxNy phases: A first-principles calculation. *Acta Materialia*, **2008**, 56, 719-725	8.4	21
152	Hyperfine interactions in hexagonal ε-Fe6Ny phase investigated by Mössbauer spectroscopy and ab initio calculations. *Acta Materialia*, **2006**, 54, 2407-2417	8.4	21
151	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	5.7	20
150	Elastic knowledge base of bcc Ti alloys from first-principles calculations and CALPHAD-based modeling. *Computational Materials Science*, **2017**, 140, 121-139	3.2	20
149	Thermodynamic modeling of fcc order/disorder transformations in the Co-Pt system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2011**, 35, 323-330	1.9	20
148	First-principles study of adsorption and diffusion of oxygen on surfaces of TiN, ZrN and HfN. *Applied Surface Science*, **2018**, 452, 457-462	6.7	20

147	Accelerating exploitation of Co-Al-based superalloys from theoretical study. *Materials and Design*, **2018**, 142, 139-148	8.1	19
146	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	1.9	19
145	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	1.9	19
144	Metastable trigonal SnP: A promising anode material for potassium-ion battery. *Carbon*, **2020**, 168, 468-474	10.4	19
143	Martensitic transition in Fe via Bain path at finite temperatures: A comprehensive first-principles study. *Acta Materialia*, **2018**, 147, 261-276	8.4	18
142	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	4.3	18
141	Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias. *Advanced Materials*, **2016**, 28, 118-23	24	18
140	Phase transformation in Ti□48Al□5Nb porous alloys and its influence on pore properties. *Materials and Design*, **2015**, 83, 508-513	8.1	17
139	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TM = Cr, Ni, Ta and Zr) alloys. *Materials Chemistry and Physics*, **2015**, 162, 748-756	4.4	17
138	Anisotropy and temperature dependence of structural, thermodynamic, and elastic properties of crystalline cellulose I□a first-principles investigation. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 085012	2	17
137	Power law scaled hardness of Mn strengthened nanocrystalline Al Mn non-equilibrium solid solutions. *Scripta Materialia*, **2016**, 120, 31-36	5.6	17
136	First-principles thermodynamic theory of Seebeck coefficients. *Physical Review B*, **2018**, 98,	3.3	17
135	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric □Mg3Sb2. *ACS Applied Energy Materials*, **2018**, 1, 6600-6608	6.1	17
134	Quantum behavior of water nano-confined in beryl. *Journal of Chemical Physics*, **2017**, 146, 124307	3.9	16
133	Understanding slow-growing alumina scale mediated by reactive elements: Perspective via local metal-oxygen bonding strength. *Scripta Materialia*, **2018**, 150, 139-142	5.6	16
132	First-principles investigation of phase stability, elastic and thermodynamic properties in L12 Co3(Al,Mo,Nb) phase. *Intermetallics*, **2016**, 78, 1-7	3.5	16
131	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	1.9	16
130	First-principles calculations and thermodynamic modeling of the Sn□r and Mg□Sn□r systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 46, 237-248	1.9	16

129	C-vacancy concentration in cementite, Fe3C1□in equilibrium with □Fe[C] and □Fe[C]. *Acta Materialia*, **2015**, 86, 374-384	8.4	16
128	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	2.3	16
127	Phonon and thermodynamic properties of Al□Mn compounds: A first-principles study. *Computational Materials Science*, **2011**, 50, 2096-2103	3.2	16
126	Phonon dispersions in random alloys: a method based on special quasi-random structure force constants. *Journal of Physics Condensed Matter*, **2011**, 23, 485403	1.8	16
125	First-principles study of binary special quasirandom structures for the Al□Cu, Al□Si, Cu□Si, and Mg□Si systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 769-773	1.9	16
124	Data set for diffusion coefficients of alloying elements in dilute Mg alloys from first-principles. *Data in Brief*, **2015**, 5, 900-12	1.2	15
123	Strengthening Mg by self-dispersed nano-lamellar faults. *Materials Research Letters*, **2017**, 5, 415-425	7.4	15
122	Thermodynamic modeling of Mg□Ca□e system by combining first-principles and CALPHAD method. *Journal of Alloys and Compounds*, **2008**, 463, 294-301	5.7	15
121	Application of the cluster variation method to □Fe2N1-z and □Fe2N: ordering of interstitial atoms. *Acta Materialia*, **2003**, 51, 3597-3606	8.4	15
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119	Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis. *APL Materials*, **2020**, 8, 081110	5.7	15
118	Revealing the Microstates of Body-Centered-Cubic (BCC) Equiatomic High Entropy Alloys. *Journal of Phase Equilibria and Diffusion*, **2017**, 38, 404-415	1	14
117	Cation Disorder Regulation by Microstate Configurational Entropy in Photovoltaic Absorber Materials Cu2ZnSn(S,Se)4. *Journal of Physical Chemistry C*, **2014**, 118, 24884-24889	3.8	14
116	Thermodynamic properties of Co3O4 and Sr6Co5O15 from first-principles. *Inorganic Chemistry*, **2010**, 49, 10291-8	5.1	14
115	Thermodynamic modelling of the B□Ca, B□Sr and B□Ba systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2007**, 31, 286-291	1.9	14
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113	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	3.2	13
112	Density Functional Theory-Based Database Development and CALPHAD Automation. *Jom*, **2013**, 65, 1533-1539	2.1	13

111	Effective elastic properties of polycrystals based on phase-field description. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2012**, 554, 67-71	5.3	13
110	Solid-Solution Hardening in Mg-Gd-TM (TM = Ag, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study. *Jom*, **2015**, 67, 2433-2441	2.1	12
109	When a defect is a pathway to improve stability: a case study of the L12 Co3TM superlattice intrinsic stacking fault. *Journal of Materials Science*, **2019**, 54, 13609-13618	4.3	12
108	Effects of alloying elements on elastic properties of Al by first-principles calculations. *Journal of Mining and Metallurgy, Section B: Metallurgy*, **2014**, 50, 37-44	1	12
107	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	1.2	12
106	Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. *Acta Materialia*, **2019**, 181, 423-438	8.4	11
105	Elastic properties of long periodic stacking ordered phases in Mg-Gd-Al alloys: A first-principles study. *Intermetallics*, **2018**, 98, 18-27	3.5	11
104	Phase stability and thermodynamic modeling of the Re□Ti system supplemented by first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2012**, 38, 71-80	1.9	11
103	Nature of ferroelectric□paraelectric transition. *Philosophical Magazine Letters*, **2012**, 92, 399-407	1	11
102	Structural mechanism for ultrahigh-strength Co-based metallic glasses. *Scripta Materialia*, **2013**, 68, 257-260	3.6	11
101	Band structure of FeBO3: Implications for tailoring the band gap of nanoparticles. *Applied Physics Letters*, **2007**, 91, 253115	3.4	11
100	The ordering behaviour of the O phase in Ti 2 AlNb-based alloys. *Intermetallics*, **2002**, 10, 979-984	3.5	11
99	Adsorption-controlled growth of Ga2O3 by suboxide molecular-beam epitaxy. *APL Materials*, **2021**, 9, 031101	5.7	11
98	On the mean kinetic energy of the proton in strong hydrogen bonded systems. *Journal of Chemical Physics*, **2016**, 144, 054302	3.9	11
97	Microstructural characteristics and crack formation in additively manufactured bimetal material of 316L stainless steel and Inconel 625. *Additive Manufacturing*, **2020**, 32, 101037	6.1	10
96	C15 NbCr2 Laves phase with mechanical properties beyond Pugh□ criterion. *Computational Materials Science*, **2016**, 121, 167-173	3.2	10
95	Synthesis, characterization and chemical stability of silicon dichalcogenides, Si(SexS1□)2. *Journal of Crystal Growth*, **2016**, 452, 151-157	1.6	10
94	Structure and energetics of Ni from ab initio molecular dynamics calculations. *Computational Materials Science*, **2014**, 89, 242-246	3.2	10

93	Quantifying charge ordering by density functional theory: Fe3O4 and CaFeO3. *Chemical Physics Letters*, **2014**, 607, 81-84	2.5	10
92	Magnetic phase transformations of face-centered cubic and hexagonal close-packed Co at zero Kelvin. *Journal of Physics Condensed Matter*, **2010**, 22, 096006	1.8	10
91	Thermodynamics of multiferroic BiFeO3: Applications for the deposition of BiFeO3 thin films. *Applied Physics Letters*, **2011**, 98, 131904	3.4	10
90	Ni3N compound layers produced by gaseous nitriding of nickel substrates; layer growth, macrostresses and intrinsic elastic anisotropy. *Journal of Materials Research*, **2012**, 27, 1531-1541	2.5	10
89	Quenching Differential Thermal Analysis and Thermodynamic Calculation to Determine Partition Coefficients of Solute Elements in Simplified Ni-Base Superalloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2010**, 41, 487-498	2.3	10
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