# Shun-Li Shang

## List of Publications by Year in Descending Order



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

| # | Paper | IF | Citations |
|---|---|---|---|
| 254 | Atomic control of active-site ensembles in ordered alloys to enhance hydrogenation selectivity.. *Nature Chemistry*, **2022**, | 17.6 | 6 |
| 253 | Predictive Crystal Plasticity Modeling of Single Crystal Nickel Based on First-Principles Calculations. *Jom*, **2022**, 74, 1423-1434 | 2.1 | 0 |
| 252 | Thermodynamic re-modelling of the CuNbSn system: Integrating the nausite phase. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2022**, 77, 102409 | 1.9 | 0 |
| 251 | Microstructure-dependent rate theory model of defect segregation and phase stability in irradiated polycrystalline LiAlO2. *Modelling and Simulation in Materials Science and Engineering*, **2022**, 30, 025005 | 2 | |
| 250 | Atomic-scale unveiling of strengthening in interstitial solid soluted Nb-rich TiAl alloys. *Journal of Alloys and Compounds*, **2022**, 917, 165484 | 5.7 | 0 |
| 249 | DFTTK: Density Functional Theory ToolKit for high-throughput lattice dynamics calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2021**, 75, 102355 | 1.9 | 4 |
| 248 | Thermodynamic properties of the Nd-Bi system via emf measurements, DFT calculations, machine learning, and CALPHAD modeling. *Acta Materialia*, **2021**, 223, 117448 | 8.4 | 3 |
| 247 | Adsorption-controlled growth of Ga2O3 by suboxide molecular-beam epitaxy. *APL Materials*, **2021**, 9, 031101 | 5.7 | 11 |
| 246 | Stability, Elastic and Electronic Properties of Ta2N by First-Principles Calculations. *Crystals*, **2021**, 11, 445 | 2.3 | 1 |
| 245 | Understanding the Effect of Oxygen on the Glass-Forming Ability of Zr55Cu55Al9Be9 Bulk Metallic Glass by ab initio Molecular Dynamics Simulations. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2021**, 52, 2501-2511 | 2.3 | 2 |
| 244 | Correlation analysis of materials properties by machine learning: illustrated with stacking fault energy from first-principles calculations in dilute fcc-based alloys. *Journal of Physics Condensed Matter*, **2021**, 33, | 1.8 | 2 |
| 243 | Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified L12 Ni3Al. *Jom*, **2021**, 73, 2285-2292 | 2.1 | 0 |
| 242 | Elastic3rd: A tool for calculating third-order elastic constants from first-principles calculations. *Computer Physics Communications*, **2021**, 261, 107777 | 4.2 | 5 |
| 241 | Underpinned exploration for magnetic structure, lattice dynamics, electronic properties, and disproportionation of yttrium nickelate. *AIP Advances*, **2021**, 11, 015028 | 1.5 | 0 |
| 240 | Understanding the surface adsorption and oxidation of cubic Cr0.5Al0.5N by first-principles calculations. *Computational Materials Science*, **2021**, 196, 110518 | 3.2 | 1 |
| 239 | Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. *Acta Materialia*, **2021**, 217, 117169 | 8.4 | 6 |
| 238 | Forming mechanism of equilibrium and non-equilibrium metallurgical phases in dissimilar aluminum/steel (Al-Fe) joints.. *Scientific Reports*, **2021**, 11, 24251 | 4.9 | 1 |

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| 237 | An ab initio molecular dynamics exploration of associates in Ba-Bi liquid with strong ordering trends. *Acta Materialia*, **2020**, 190, 81-92 | 8.4 | 3 |
| 236 | High-throughput investigations of configurational-transformation-dominated serrations in CuZr/Cu nanolaminates. *Journal of Materials Science and Technology*, **2020**, 53, 192-199 | 9.1 | 9 |
| 235 | A brief review of data-driven ICME for intelligently discovering advanced structural metal materials: Insight into atomic and electronic building blocks. *Journal of Materials Research*, **2020**, 35, 872-889 | 2.5 | 8 |
| 234 | Unveiling dislocation characteristics in Ni3Al from stacking fault energy and ideal strength: A first-principles study via pure alias shear deformation. *Physical Review B*, **2020**, 101, | 3.3 | 7 |
| 233 | An orthorhombic D022-like precursor to Al8Mo3 in the Al□Mo□i system. *Journal of Alloys and Compounds*, **2020**, 823, 153807 | 5.7 | 4 |
| 232 | 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 |
| 231 | Anomalous phonon-mode dependence in polarized Raman spectroscopy of the topological Weyl semimetal TaP. *Physical Review B*, **2020**, 101, | 3.3 | 3 |
| 230 | Anisotropic Fano resonance in the Weyl semimetal candidate LaAlSi. *Physical Review B*, **2020**, 102, | 3.3 | 6 |
| 229 | Metastable trigonal SnP: A promising anode material for potassium-ion battery. *Carbon*, **2020**, 168, 468-474 | 10.4 | 19 |
| 228 | Unveiling non-equilibrium metallurgical phases in dissimilar Al-Cu joints processed by vaporizing foil actuator welding. *Materials and Design*, **2020**, 186, 108306 | 8.1 | 15 |
| 227 | Realization of Epitaxial Thin Films of the Topological Crystalline Insulator Sr SnO. *Advanced Materials*, **2020**, 32, e2000809 | 24 | 8 |
| 226 | Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis. *APL Materials*, **2020**, 8, 081110 | 5.7 | 15 |
| 225 | Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. *Computational Materials Science*, **2020**, 171, 109263 | 3.2 | 3 |
| 224 | Diffusion of hydrogen isotopes in 3C-SiC in HTR-PM: A first-principles study. *Progress in Nuclear Energy*, **2020**, 119, 103181 | 2.3 | 0 |
| 223 | Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. *Acta Materialia*, **2019**, 181, 423-438 | 8.4 | 11 |
| 222 | An alternative approach to predict Seebeck coefficients: Application to La3□Te4. *Scripta Materialia* , **2019**, 169, 87-91 | 5.6 | 7 |
| 221 | Thermodynamic modeling of the Si-Y system aided by first-principles and phonon calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2019**, 65, 282-290 | 1.9 | 4 |
| 220 | High Performance Anion Exchange Membrane Fuel Cells Enabled by Fluoropoly(olefin) Membranes. *Advanced Functional Materials*, **2019**, 29, 1902059 | 15.6 | 72 |

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|---|---|---|---|
| 219 | Local lattice distortion mediated formation of stacking faults in Mg alloys. *Acta Materialia*, **2019**, 170, 231-239 | 8.4 | 23 |
| 218 | Experimental isothermal section of the Nb-Ni-Ru ternary system at 1100 °C. *Journal of Alloys and Compounds*, **2019**, 810, 151801 | 5.7 | 1 |
| 217 | 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 |
| 216 | The stability of deformation twins in aluminum enhanced by alloying elements. *Journal of Materials Science and Technology*, **2019**, 35, 2625-2629 | 9.1 | 5 |
| 215 | Effects of Hf, Y, and Zr on Alumina Scale Growth on NiAlCr and NiAlPt Alloys. *Oxidation of Metals*, **2019**, 92, 303-313 | 1.6 | 8 |
| 214 | Study on impact of Cr and Mo on diffusion of H in 2.25Cr1Mo steel using first-principle calculations. *Journal of Nuclear Materials*, **2019**, 525, 152-160 | 3.3 | 2 |
| 213 | Phase equilibria of Ti-Al-V system at 1300 °C. *Intermetallics*, **2019**, 115, 106609 | 3.5 | 4 |
| 212 | Achieving accurate energetics beyond (semi-)local density functional theory: Illustrated with transition metal disulfides, Cu2ZnSnS4, and Na3PS4 related semiconductors. *Physical Review Materials*, **2019**, 3, | 3.2 | 4 |
| 211 | Thermodynamic properties and phase stability of the Ba-Bi system: A combined computational and experimental study. *Journal of Alloys and Compounds*, **2019**, 771, 281-289 | 5.7 | 3 |
| 210 | 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 |
| 209 | A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields. *Nature Nanotechnology*, **2019**, 14, 131-136 | 28.7 | 98 |
| 208 | From random stacking faults to polytypes: A 12-layer NiSn4 polytype. *Journal of Alloys and Compounds*, **2019**, 774, 265-273 | 5.7 | 1 |
| 207 | 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 |
| 206 | Synthesis science of SrRuO3 and CaRuO3 epitaxial films with high residual resistivity ratios. *APL Materials*, **2018**, 6, 046101 | 5.7 | 41 |
| 205 | First-principles calculations of lattice dynamics and thermodynamic properties for Yb14MnSb11. *Journal of Applied Physics*, **2018**, 123, 045102 | 2.5 | 8 |
| 204 | A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8. *Nano Energy*, **2018**, 47, 325-330 | 17.1 | 45 |
| 203 | Martensitic transition in Fe via Bain path at finite temperatures: A comprehensive first-principles study. *Acta Materialia*, **2018**, 147, 261-276 | 8.4 | 18 |
| 202 | Accelerating exploitation of Co-Al-based superalloys from theoretical study. *Materials and Design*, **2018**, 142, 139-148 | 8.1 | 19 |

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| 201 | 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 |
| 200 | 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 |
| 199 | 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 |
| 198 | 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 |
| 197 | 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 |
| 196 | Effect of alloying elements on the stacking fault energies of dilute al-based alloys. *Journal of Mining and Metallurgy, Section B: Metallurgy*, **2018**, 54, 185-196 | 1 | 5 |
| 195 | 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 |
| 194 | Quasiharmonic calculations of thermodynamic properties for La3Te4 system. *Computational Materials Science*, **2018**, 142, 417-426 | 3.2 | 5 |
| 193 | First-principles calculations and thermodynamic modelling of long periodic stacking ordered (LPSO) phases in Mg-Al-Gd. *Materialia*, **2018**, 4, 192-202 | 3.2 | 4 |
| 192 | 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 |
| 191 | First-principles thermodynamic theory of Seebeck coefficients. *Physical Review B*, **2018**, 98, | 3.3 | 17 |
| 190 | Thermodynamic Assessment of the Ag-Se System Aided by First-Principles Calculations. *Journal of Phase Equilibria and Diffusion*, **2018**, 39, 870-881 | 1 | 1 |
| 189 | Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Mg3Sb2. *ACS Applied Energy Materials*, **2018**, 1, 6600-6608 | 6.1 | 17 |
| 188 | A first-principles based description of the Hf-Ni system supported by high-temperature synchrotron experiments. *Thermochimica Acta*, **2018**, 668, 142-151 | 2.9 | 4 |
| 187 | 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 |
| 186 | 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 |
| 185 | Phase stability, elastic, and thermodynamic properties of the L12 (Co,Ni)3(Al,Mo,Nb) phase from first-principles calculations. *Journal of Materials Research*, **2017**, 32, 2100-2108 | 2.5 | 6 |
| 184 | Origin of Outstanding Phase and Moisture Stability in a NaPAsS Superionic Conductor. *ACS Applied Materials & Interfaces*, **2017**, 9, 16261-16269 | 9.5 | 38 |

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| 183 | Revealing the Microstates of Body-Centered-Cubic (BCC) Equiatomic High Entropy Alloys. *Journal of Phase Equilibria and Diffusion*, **2017**, 38, 404-415 | 1 | 14 |
| 182 | Quantum behavior of water nano-confined in beryl. *Journal of Chemical Physics*, **2017**, 146, 124307 | 3.9 | 16 |
| 181 | First-principles calculations and thermodynamic modeling of the Sn-Ta system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2017**, 57, 46-54 | 1.9 | 3 |
| 180 | Thermodynamic modeling of phase equilibria and defect chemistry in the Zn-S system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2017**, 59, 171-181 | 1.9 | 6 |
| 179 | A curved pathway for oxygen interstitial diffusion in aluminum. *Computational Materials Science*, **2017**, 140, 47-54 | 3.2 | 8 |
| 178 | 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 |
| 177 | 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 |
| 176 | Insight into □Ni/□-Ni3Al interfacial energy affected by alloying elements. *Materials and Design*, **2017**, 133, 39-46 | 8.1 | 21 |
| 175 | Atomic and electronic basis for the serrations of refractory high-entropy alloys. *Npj Computational Materials*, **2017**, 3, | 10.9 | 39 |
| 174 | Strengthening Mg by self-dispersed nano-lamellar faults. *Materials Research Letters*, **2017**, 5, 415-425 | 7.4 | 15 |
| 173 | First-principles calculations and thermodynamic modeling of the S-Se system and implications for chalcogenide alloys. *Journal of Alloys and Compounds*, **2017**, 694, 510-521 | 5.7 | 6 |
| 172 | Fundamentals of Thermal Expansion and Thermal Contraction. *Materials*, **2017**, 10, | 3.5 | 9 |
| 171 | Adsorption-controlled growth of La-doped BaSnO3 by molecular-beam epitaxy. *APL Materials*, **2017**, 5, 116107 | 5.7 | 98 |
| 170 | Lateral Versus Vertical Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides: Thermodynamic Insight into MoS2. *Nano Letters*, **2016**, 16, 5742-50 | 11.5 | 70 |
| 169 | Lattice dynamics, thermodynamics and elastic properties of C22-Zr6FeSn2 from first-principles calculations. *Journal of Nuclear Materials*, **2016**, 479, 461-469 | 3.3 | 8 |
| 168 | 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 |
| 167 | Fabrication of nano-porous □Al2O3 layers on porous Ti-48Al-6Nb alloys. *Materials and Design*, **2016**, 109, 700-708 | 8.1 | 6 |
| 166 | Stacking disorder in metastable NiSn4. *Materials and Design*, **2016**, 109, 324-333 | 8.1 | 7 |

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| 165 | First-principles calculations of lattice dynamics and thermal properties of polar solids. *Npj Computational Materials*, **2016**, 2, | 10.9 | 88 |
| 164 | Solid Solution Hardening in Mg-Gd-TM (TM=Ag, Zn and Zr) Alloys: an Integrated Density Functional Theory and Electron Work Function Study **2016**, 155-157 | | |
| 163 | C15 NbCr2 Laves phase with mechanical properties beyond Pugh□ criterion. *Computational Materials Science*, **2016**, 121, 167-173 | 3.2 | 10 |
| 162 | Thermodynamics of the S□n system: Implication for synthesis of earth abundant photovoltaic absorber materials. *Solar Energy*, **2016**, 125, 314-323 | 6.8 | 27 |
| 161 | Synthesis, characterization and chemical stability of silicon dichalcogenides, Si(SexS1□)2. *Journal of Crystal Growth*, **2016**, 452, 151-157 | 1.6 | 10 |
| 160 | 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 |
| 159 | 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 |
| 158 | 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 |
| 157 | Diffusion coefficients of alloying elements in dilute Mg alloys: A comprehensive first-principles study. *Acta Materialia*, **2016**, 103, 573-586 | 8.4 | 108 |
| 156 | Solid Solution Hardening in Mg-Gd-TM (TM=Ag, Zn and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study **2016**, 157-157 | | |
| 155 | First-principles Study of Diffusion Coefficients of Alloy Elements in Dilute Mg Alloys **2016**, 97-101 | | |
| 154 | On the mean kinetic energy of the proton in strong hydrogen bonded systems. *Journal of Chemical Physics*, **2016**, 144, 054302 | 3.9 | 11 |
| 153 | Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias. *Advanced Materials*, **2016**, 28, 118-23 | 24 | 18 |
| 152 | Ferromagnetism: Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias (Adv. Mater. 1/2016). *Advanced Materials*, **2016**, 28, 204-204 | 24 | |
| 151 | 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 |
| 150 | Generalization of first-principles thermodynamic model: Application to hexagonal close-packed □Fe3N. *Computational Materials Science*, **2016**, 117, 83-89 | 3.2 | 4 |
| 149 | Power law scaled hardness of Mn strengthened nanocrystalline Al Mn non-equilibrium solid solutions. *Scripta Materialia*, **2016**, 120, 31-36 | 5.6 | 17 |
| 148 | A New Relationship Among Self- and Impurity Diffusion Coefficients in Binary Solution Phases. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2016**, 47, 3295-3299 | 2.3 | 3 |

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| 147 | First-principles Study of Diffusion Coefficients of Alloy Elements in Dilute Mg Alloys **2016**, 97-101 | | |
| 146 | Prediction of Diffusion Coefficients in Liquid and Solids. *Defect and Diffusion Forum*, **2015**, 364, 182-191 | 0.7 | 9 |
| 145 | Phase transformation in Ti48Al8Nb porous alloys and its influence on pore properties. *Materials and Design*, **2015**, 83, 508-513 | 8.1 | 17 |
| 144 | Mechanical properties and spinodal decomposition of TixAl1−x−yZryN coatings. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2015**, 379, 2037-2040 | 2.3 | 2 |
| 143 | Ti-substituted Li[Li0.26Mn0.67TixNi0.07Co0.07]O2 layered cathode material with improved structural stability and suppressed voltage fading. *Journal of Materials Chemistry A*, **2015**, 3, 17376-17384 | 13 | 33 |
| 142 | A novel hot pack rolling of high Nb-TiAl sheet from cast ingot. *Intermetallics*, **2015**, 67, 19-25 | 3.5 | 33 |
| 141 | Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study. *Acta Materialia*, **2015**, 97, 75-85 | 8.4 | 46 |
| 140 | Deformation behaviour and 6H-LPSO structure formation at nanoindentation in lamellar high Nb containing TiAl alloy. *Philosophical Magazine Letters*, **2015**, 95, 85-91 | 1 | 7 |
| 139 | Elastic anisotropy of iron carbides with trigonal-prismatic coordination of C by Fe. *Journal of Alloys and Compounds*, **2015**, 633, 390-394 | 5.7 | 8 |
| 138 | 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 |
| 137 | Thermodynamic Modeling of the Pt-Te and Pt-Sb-Te Systems. *Journal of Electronic Materials*, **2015**, 44, 2638-2650 | 1.9 | 5 |
| 136 | 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 |
| 135 | Strain-induced dimensionality crossover of precursor modulations in Ni2MnGa. *Applied Physics Letters*, **2015**, 106, 021910 | 3.4 | 3 |
| 134 | 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 |
| 133 | Thermodynamic modeling of the CaO-CaF2-Al2O3 system aided by first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2015**, 48, 113-122 | 1.9 | 9 |
| 132 | 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 |
| 131 | Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. *Acta Materialia*, **2015**, 82, 287-294 | 8.4 | 23 |
| 130 | Crystal structure and phase stability of AlSc in the near-equiatomic Al-Sc alloy. *Journal of Alloys and Compounds*, **2015**, 618, 192-196 | 5.7 | 2 |

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|---|---|---|---|
| 129 | 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 |
| 128 | Nb–Al diffusion reaction in high Nb containing TiAl porous alloys. *Materials Science and Technology*, **2015**, 31, 1388-1391 | 1.5 | 8 |
| 127 | Impact of W on structural evolution and diffusivity of Ni–W melts: an ab initio molecular dynamics study. *Journal of Materials Science*, **2015**, 50, 1071-1081 | 4.3 | 7 |
| 126 | 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 |
| 125 | C-vacancy concentration in cementite, Fe3C1−δ, in equilibrium with γ-Fe[C] and α-Fe[C]. *Acta Materialia*, **2015**, 86, 374-384 | 8.4 | 16 |
| 124 | Nature of ferroelectric-paraelectric phase transition and origin of negative thermal expansion in PbTiO3. *Physical Review B*, **2015**, 91, | 3.3 | 25 |
| 123 | Thermal expansion anomaly regulated by entropy. *Scientific Reports*, **2014**, 4, 7043 | 4.9 | 46 |
| 122 | Vacancy mechanism of oxygen diffusivity in bcc Fe: A first-principles study. *Corrosion Science*, **2014**, 83, 94-102 | 6.8 | 47 |
| 121 | A first-principles study of self-diffusion coefficients of fcc Ni. *Computational Materials Science*, **2014**, 86, 17-23 | 3.2 | 27 |
| 120 | Reaction behavior and pore formation mechanism of TiAl–Nb porous alloys prepared by elemental powder metallurgy. *Intermetallics*, **2014**, 44, 1-7 | 3.5 | 32 |
| 119 | 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 |
| 118 | Temperature-dependent elastic stiffness constants of fcc-based metal nitrides from first-principles calculations. *Journal of Materials Science*, **2014**, 49, 424-432 | 4.3 | 8 |
| 117 | First-principles study of the mechanical properties and phase stability of TiO2. *Computational Materials Science*, **2014**, 83, 114-119 | 3.2 | 26 |
| 116 | First-principles calculations of finite-temperature thermodynamic properties of binary solid solutions in the Al–Cu–Mg system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 47, 196-210 | 1.9 | 7 |
| 115 | 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 |
| 114 | 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 |
| 113 | First-principles calculations and thermodynamic modeling of the Sn–Sr and Mg–Sn–Sr systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 46, 237-248 | 1.9 | 16 |
| 112 | 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 |

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|---|---|---|---|
| 111 | 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 |
| 110 | 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 |
| 109 | Structure and energetics of Ni from ab initio molecular dynamics calculations. *Computational Materials Science*, **2014**, 89, 242-246 | 3.2 | 10 |
| 108 | Quantifying charge ordering by density functional theory: Fe3O4 and CaFeO3. *Chemical Physics Letters*, **2014**, 607, 81-84 | 2.5 | 10 |
| 107 | Thermodynamic modeling of the In□Pt□Sb system. *International Journal of Materials Research*, **2014**, 105, 525-536 | 0.5 | 2 |
| 106 | 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 |
| 105 | Thermodynamic description of the Ta□V□Zr system. *International Journal of Materials Research*, **2014**, 105, 1048-1056 | 0.5 | 5 |
| 104 | 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 |
| 103 | A new many-body potential with the second-moment approximation of tight-binding scheme for Hafnium. *Science China: Physics, Mechanics and Astronomy*, **2013**, 56, 2071-2080 | 3.6 | |
| 102 | Density Functional Theory-Based Database Development and CALPHAD Automation. *Jom*, **2013**, 65, 1533-1539 | 2.1 | 13 |
| 101 | Thermodynamic properties of magnesium alloys **2013**, 85-124 | | |
| 100 | Pore structure and gas permeability of high Nb-containing TiAl porous alloys by elemental powder metallurgy for microfiltration application. *Intermetallics*, **2013**, 33, 2-7 | 3.5 | 32 |
| 99 | BiFeO3 domain wall energies and structures: a combined experimental and density functional theory+U study. *Physical Review Letters*, **2013**, 110, 267601 | 7.4 | 49 |
| 98 | Structural mechanism for ultrahigh-strength Co-based metallic glasses. *Scripta Materialia*, **2013**, 68, 257-260 | 3.6 | 11 |
| 97 | Accurate calculations of phonon dispersion in CaF2 and CeO2. *Physical Review B*, **2013**, 88, | 3.3 | 21 |
| 96 | Low energy structures of lithium-ion battery materials Li(MnxNixCo1□x)O2 revealed by first-principles calculations. *Applied Physics Letters*, **2013**, 103, 053903 | 3.4 | 9 |
| 95 | 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 |
| 94 | 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 |

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