Zi-Kui Liu

List of Publications by Year
in descending order

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596	26,147	8755	15698
papers	citations	77 h-index	129 g-index

618	618	618	20815
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ordering in liquid and its heredity impact on phase transformation of Mg-Al-Ca alloys. Journal of Magnesium and Alloys, 2023, 11, 2006-2017.	5.5	12
2	Thermodynamic properties of the Nd-Bi system via emf measurements, DFT calculations, machine learning, and CALPHAD modeling. Acta Materialia, 2022, 223, 117448.	3.8	10
3	Thermodynamic modeling of the Al-Co-Cr-Fe-Ni high entropy alloys supported by key experiments. Journal of Alloys and Compounds, 2022, 897, 162722.	2.8	10
4	Design of an additively manufactured functionally graded material of 316 stainless steel and Ti-6Al-4V with Ni-20Cr, Cr, and V intermediate compositions. Additive Manufacturing, 2022, 51, 102649.	1.7	7
5	Atomic control of active-site ensembles in ordered alloys to enhance hydrogenation selectivity. Nature Chemistry, 2022, 14, 523-529.	6.6	51
6	Zentropy Theory for Positive and Negative Thermal Expansion. Journal of Phase Equilibria and Diffusion, 2022, 43, 598-605.	0.5	17
7	Predictive Crystal Plasticity Modeling of Single Crystal Nickel Based on First-Principles Calculations. Jom, 2022, 74, 1423-1434.	0.9	2
8	Thermodynamic re-modelling of the Cuâ€“Nbâ€“Sn system: Integrating the nausite phase. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102409.	0.7	4
9	Extensible Structure-Informed Prediction of Formation Energy with improved accuracy and usability employing neural networks. Computational Materials Science, 2022, 208, 111254.	1.4	17
10	Theory of cross phenomena and their coefficients beyond Onsager theorem. Materials Research Letters, 2022, 10, 393-439.	4.1	46
11	Atomic-scale unveiling of strengthening in interstitial solid soluted Nb-rich TiAl alloys. Journal of Alloys and Compounds, 2022, 917, 165484.	2.8	8
12	Electrochemical recovery of Nd using liquid metals (Bi and Sn) in LiCl-KCl-NdCl3. Electrochimica Acta, 2022, 425, 140655.	2.6	11
13	Insight into ideal shear strength of Ni-based dilute alloys using first-principles calculations and correlational analysis. Computational Materials Science, 2022, 212, 111564.	1.4	1
14	Enhancing Moisture Stability of Sulfide Solid-State Electrolytes by Reversible Amphipathic Molecular Coating. ACS Applied Materials & Interfaces, 2022, 14, 32035-32042.	4.0	5
15	Elastic3rd: A tool for calculating third-order elastic constants from first-principles calculations. Computer Physics Communications, 2021, 261, 107777.	3.0	22
16	Integrating data mining and machine learning to discover high-strength ductile titanium alloys. Acta Materialia, 2021, 202, 211-221.	3.8	85
17	Underpinned exploration for magnetic structure, lattice dynamics, electronic properties, and disproportionation of yttrium nickelate. AIP Advances, 2021, 11, .	0.6	5
18	Adsorption-controlled growth of Ga2O3 by suboxide molecular-beam epitaxy. APL Materials, 2021, 9, .	2.2	38

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19	Plasticity and fracture behavior of Inconel 625 manufactured by laser powder bed fusion: Comparison between as-built and stress relieved conditions. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2021, 806, 140808.	2.6	19
20	Stability, Elastic and Electronic Properties of Ta2N by First-Principles Calculations. Crystals, 2021, 11, 445.	1.0	3
21	Effect of processing parameters and strut dimensions on the microstructures and hardness of stainless steel 316L lattice-emulating structures made by powder bed fusion. Additive Manufacturing, 2021, 40, 101943.	1.7	6
22	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.	1.1	6
23	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, 295702.	0.7	13
24	Preferential uptake of antibody targeted calcium phosphosilicate nanoparticles by metastatic triple negative breast cancer cells in co-cultures of human metastatic breast cancer cells plus bone osteoblasts. Nanomedicine: Nanotechnology, Biology, and Medicine, 2021, 34, 102383.	1.7	5
25	Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified L12 Ni3Al. Jom, 2021, 73, 2285-2292.	0.9	2
26	Comment on â€œThermodiffusion: The physico-chemical mechanics viewâ€•[J. Chem. Phys. 154, 024112 (2021)]. Journal of Chemical Physics, 2021, 155, 087101.	1.2	8
27	Understanding the surface adsorption and oxidation of cubic Cr0.5Al0.5N by first-principles calculations. Computational Materials Science, 2021, 196, 110518.	1.4	6
28	Revisiting the third-order elastic constants of diamond: The higher-order effect. Diamond and Related Materials, 2021, 117, 108490.	1.8	9
29	Tensile behavior of stainless steel 304L to Ni-20Cr functionally graded material: Experimental characterization and computational simulations. Materialia, 2021, 18, 101151.	1.3	14
30	Preparation of CoGe2-type NiSn2 at 10ÂGPa. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2021, .	0.3	0
31	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. Acta Materialia, 2021, 217, 117169.	3.8	34
32	Searching for a route to synthesize in situ epitaxial Pr2Ir2O7 thin films with thermodynamic methods. Npj Computational Materials, 2021, 7, .	3.5	4
33	Corrosion behavior in aluminum/galvanized steel resistance spot welds and self-piercing riveting joints in salt spray environment. Journal of Manufacturing Processes, 2021, 70, 608-620.	2.8	15
34	Sensitivity estimation for calculated phase equilibria. Journal of Materials Research, 2021, 36, 140-150.	1.2	11
35	Atomic structure, diffusivity and viscosity of Al1-xMgx melts from ab initio molecular dynamics simulations. Journal of Mining and Metallurgy, Section B: Metallurgy, 2021, 57, 31-40.	0.3	1
36	Exact phenomenological theory for thermotransport in a solid binary alloy. Philosophical Magazine Letters, 2021, 101, 123-131.	0.5	2

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37	Sensitivity estimation for calculated phase equilibria. Journal of Materials Research, 2021, 36, 1-11.	1.2	1
38	DFTTK: Density Functional Theory ToolKit for high-throughput lattice dynamics calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 75, 102355.	0.7	17
39	Ab initio simulations on the pure Cr lattice stability at 0K: Verification with the Fe-Cr and Ni-Cr binary systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 75, 102359.	0.7	14
40	Forming mechanism of equilibrium and non-equilibrium metallurgical phases in dissimilar aluminum/steel (Alâ€“Fe) joints. Scientific Reports, 2021, 11, 24251.	1.6	8
41	Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. Computational Materials Science, 2020, 171, 109263.	1.4	5
42	Diffusion of hydrogen isotopes in 3C-SiC in HTR-PM: A first-principles study. Progress in Nuclear Energy, 2020, 119, 103181.	1.3	2
43	Analysis of formation and growth of the Ïƒ phase in additively manufactured functionally graded materials. Journal of Alloys and Compounds, 2020, 814, 151729.	2.8	28
44	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
45	Measurement of interdiffusivity for fcc_A1 Co-V-W alloys. International Journal of Refractory Metals and Hard Materials, 2020, 87, 105134.	1.7	3
46	Solute effects on the Ï£3 <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mfenced open="(") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 397 Td (close=")"><mml:mrow><mml:mr stretchy="false">[</mml:mo><mml:mn>1</mml:mn><mml:mover accent="true"><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:mover><mm stretchy="false">]</mml:mo></mml:mrow></mml:mrow></mml:math> tilt grain boundary in BCC Fe: Gr	1.4	37
47	Computational thermodynamics and its applications. Acta Materialia, 2020, 200, 745-792.	3.8	91
48	Realization of Epitaxial Thin Films of the Topological Crystalline Insulator Sr 3 SnO. Advanced Materials, 2020, 32, 2000809.	11.1	15
49	Experimental and computational studies of melting of the spinel phase in the Feâ€“Alâ€“O ternary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 70, 101798.	0.7	2
50	Statistical approach for automated weighting of datasets: Application to heat capacity data. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 71, 101994.	0.7	7
51	Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis. APL Materials, 2020, 8, .	2.2	28
52	An ab initio molecular dynamics exploration of associates in Ba-Bi liquid with strong ordering trends. Acta Materialia, 2020, 190, 81-92.	3.8	13
53	High-throughput investigations of configurational-transformation-dominated serrations in CuZr/Cu nanolaminates. Journal of Materials Science and Technology, 2020, 53, 192-199.	5.6	14
54	Thermodynamic re-assessment of pure chromium using modified segmented regression model. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 69, 101762.	0.7	8

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55	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. Engineering, 2020, 6, 612-620.	3.2	4
56	View and Comments on the Data Ecosystem: â€œOcean of Dataâ€• Engineering, 2020, 6, 604-608.	3.2	2
57	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.	1.2	17
58	Experimental phase diagram, thermodynamic modeling and solidified microstructure in the Moâ€“Niâ€“W ternary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 68, 101748.	0.7	14
59	Experimental validation of Scheilâ€“Gulliver simulations for gradient path planning in additively manufactured functionally graded materials. Materialia, 2020, 11, 100689.	1.3	36
60	Freestanding ultra-thin silica. AIP Advances, 2020, 10, 025126.	0.6	1
61	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
62	An orthorhombic D022-like precursor to Al8Mo3 in the Alâ€“Moâ€“Ti system. Journal of Alloys and Compounds, 2020, 823, 153807.	2.8	7
63	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
64	Anomalous phonon-mode dependence in polarized Raman spectroscopy of the topological Weyl semimetal TaP. Physical Review B, 2020, 101, .	1.1	8
65	Metastable trigonal SnP: A promising anode material for potassium-ion battery. Carbon, 2020, 168, 468-474.	5.4	32
66	Anisotropic Fano resonance in the Weyl semimetal candidate LaAlSi. Physical Review B, 2020, 102, .	1.1	16
67	Thermodynamic Properties of Srâ€“Sn Alloys via Emf Measurements and Thermal Analysis. Journal of the Electrochemical Society, 2020, 167, 082508.	1.3	3
68	Experimental isothermal section of the Nb-Ni-Ru ternary system at 1100â€Â°C. Journal of Alloys and Compounds, 2019, 810, 151801.	2.8	2
69	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.	1.7	16
70	Atomic mobility evaluation and diffusion matrix for fcc_A1 Coâ€“Vâ€“W alloys. Journal of Materials Science, 2019, 54, 13420-13432.	1.7	7
71	Effects of Hf, Y, and Zr on Alumina Scale Growth on NiAlCr and NiAlPt Alloys. Oxidation of Metals, 2019, 92, 303-313.	1.0	15
72	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.	1.3	3

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73	ESPEI for efficient thermodynamic database development, modification, and uncertainty quantification: application to Cuâ€“Mg. MRS Communications, 2019, 9, 618-627.	0.8	49
74	Phase equilibria of Tiâ€“Alâ€“V system at 1300â€¯Â°C. Intermetallics, 2019, 115, 106609.	1.8	5
75	Sintering mechanism of Cu-9Al alloy prepared from elemental powders. Progress in Natural Science: Materials International, 2019, 29, 425-431.	1.8	9
76	Local electronic descriptors for solute-defect interactions in bcc refractory metals. Nature Communications, 2019, 10, 4484.	5.8	19
77	Microstructure, mechanical properties and cutting performances of TiSiCN super-hard nanocomposite coatings deposited using CVD method under the guidance of thermodynamic calculations. Surface and Coatings Technology, 2019, 378, 124956.	2.2	16
78	Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. Acta Materialia, 2019, 181, 423-438.	3.8	18
79	An alternative approach to predict Seebeck coefficients: Application to La3â^'xTe4. Scripta Materialia, 2019, 169, 87-91.	2.6	9
80	Multiscale Entropy and Its Implications to Critical Phenomena, Emergent Behaviors, and Information. Journal of Phase Equilibria and Diffusion, 2019, 40, 508-521.	0.5	17
81	High-throughput thermodynamic calculations of phase equilibria in solidified 6016 Al-alloys. Computational Materials Science, 2019, 167, 19-24.	1.4	18
82	Multipoint Defect Synergy Realizing the Excellent Thermoelectric Performance of nâ€Type Polycrystalline SnSe via Re Doping. Advanced Functional Materials, 2019, 29, 1902893.	7.8	73
83	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.	0.7	7
84	High Performance Anion Exchange Membrane Fuel Cells Enabled by Fluoropoly(olefin) Membranes. Advanced Functional Materials, 2019, 29, 1902059.	7.8	128
85	Quantified uncertainty in thermodynamic modeling for materials design. Acta Materialia, 2019, 174, 9-15.	3.8	40
86	Computer simulation of thermodynamic factors in Ni-Al and Cu-Ag liquid alloys. Computational Materials Science, 2019, 166, 124-135.	1.4	3
87	Local lattice distortion mediated formation of stacking faults in Mg alloys. Acta Materialia, 2019, 170, 231-239.	3.8	45
88	First-principles lattice dynamics and thermodynamic properties of pre-perovskite PbTiO3. Acta Materialia, 2019, 171, 146-153.	3.8	11
89	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.	2.8	4
90	Mass and thermal transport in liquid Cu-Ag alloys. Philosophical Magazine, 2019, 99, 468-491.	0.7	10

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91	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
92	Integrated computational materials engineering for advanced materials: A brief review. Computational Materials Science, 2019, 158, 42-48.	1.4	84
93	A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields. Nature Nanotechnology, 2019, 14, 131-136.	15.6	150
94	From random stacking faults to polytypes: A 12-layer NiSn4 polytype. Journal of Alloys and Compounds, 2019, 774, 265-273.	2.8	4
95	Achieving accurate energetics beyond (semi-)local density functional theory: Illustrated with transition metal disulfides, Cu2ZnSnS4 , and Na3PS4 related semiconductors. Physical Review Materials, 2019, 3, .	0.9	6
96	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
97	Synthesis science of SrRuO3 and CaRuO3 epitaxial films with high residual resistivity ratios. APL Materials, 2018, 6, .	2.2	61
98	First-principles calculations of lattice dynamics and thermodynamic properties for Yb14MnSb11. Journal of Applied Physics, 2018, 123, .	1.1	10
99	A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8. Nano Energy, 2018, 47, 325-330.	8.2	55
100	Martensitic transition in Fe via Bain path at finite temperatures: A comprehensive first-principles study. Acta Materialia, 2018, 147, 261-276.	3.8	44
101	Characterization of a functionally graded material of Ti-6Al-4V to 304L stainless steel with an intermediate V section. Journal of Alloys and Compounds, 2018, 742, 1031-1036.	2.8	89
102	Powder chemistry effects on the sintering of MgOâ€doped specialty Al₂O₃. Journal of the American Ceramic Society, 2018, 101, 2739-2751.	1.9	4
103	Î±-SnSe thin film solar cells produced by selenization of magnetron sputtered tin precursors. Solar Energy Materials and Solar Cells, 2018, 176, 251-258.	3.0	27
104	Accelerating exploitation of Co-Al-based superalloys from theoretical study. Materials and Design, 2018, 142, 139-148.	3.3	29
105	Electrically reversible cracks in an intermetallic film controlled by an electric field. Nature Communications, 2018, 9, 41.	5.8	53
106	Deposition of CVD-TiCN and TiAlN coatings guided with thermodynamic calculations. International Journal of Materials Research, 2018, 109, 277-283.	0.1	12
107	The Thermodynamic Database Database. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 173-178.	0.7	25
108	Experimental Determination of Impurity and Interdiffusion Coefficients in Seven Ti and Zr Binary Systems Using Diffusion Multiples. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2018, 49, 3108-3116.	1.1	24

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109	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
110	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
111	Phase stability and mechanical properties of AlHfNbTiZr high-entropy alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 724, 249-259.	2.6	67
112	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
113	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
114	High thermoelectric performance of few-quintuple Sb2Te3 nanofilms. Nano Energy, 2018, 43, 285-290.	8.2	51
115	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
116	Superâ€High Strength Mgâ€“7.5Alâ€“0.8Zn Alloy Prepared by Rapidly Solidified Powder Metallurgy and Low Temperature Extrusion. Advanced Engineering Materials, 2018, 20, 1700712.	1.6	1
117	Quasiharmonic calculations of thermodynamic properties for La3â^'xTe4 system. Computational Materials Science, 2018, 142, 417-426.	1.4	6
118	Design of Materials Processing Using Computational Thermodynamics. , 2018, , 27-45.		0
119	A hybrid functional study of native point defects in Cu₂SnS₃: implications for reducing carrier recombination. Physical Chemistry Chemical Physics, 2018, 20, 256-261.	1.3	12
120	Phase field simulation of the phase separation in the TiC-ZrC-WC system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 63, 190-195.	0.7	27
121	First-principles calculations and thermodynamic modelling of long periodic stacking ordered (LPSO) phases in Mg-Al-Gd. Materialia, 2018, 4, 192-202.	1.3	8
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	First-principles thermodynamic theory of Seebeck coefficients. Physical Review B, 2018, 98, .	1.1	25
124	Thermodynamic Assessment of the Ag-Se System Aided by First-Principles Calculations. Journal of Phase Equilibria and Diffusion, 2018, 39, 870-881.	0.5	2
125	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Î±-Mg₃Sb₂. ACS Applied Energy Materials, 2018, 1, 6600-6608.	2.5	28
126	Control of Epitaxial BaFe₂As₂ Atomic Configurations with Substrate Surface Terminations. Nano Letters, 2018, 18, 6347-6352.	4.5	16

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127	A first-principles based description of the Hf-Ni system supported by high-temperature synchrotron experiments. Thermochimica Acta, 2018, 668, 142-151.	1.2	9
128	Thermodynamic modeling of the La-Te system aided by first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 61, 227-236.	0.7	4
129	Experimental analysis and thermodynamic calculations of an additively manufactured functionally graded material of V to Invar 36. Journal of Materials Research, 2018, 33, 1642-1649.	1.2	20
130	Ocean of Data: Integrating First-Principles Calculations and CALPHAD Modeling with Machine Learning. Journal of Phase Equilibria and Diffusion, 2018, 39, 635-649.	0.5	27
131	Synergistic Effects of Nano-ZnO and Low pH of Sea Water on the Physiological Energetics of the Thick Shell Mussel Mytilus coruscus. Frontiers in Physiology, 2018, 9, 757.	1.3	22
132	On Sluggish Diffusion in Fcc Alâ€“Coâ€“Crâ€“Feâ€“Ni High-Entropy Alloys: An Experimental and Numerical Study. Metals, 2018, 8, 16.	1.0	62
133	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
134	Revisiting the Phase Stability in Ni-X (X=Mo, Ti, In) Systems Using Ab Initio Calculations. Journal of Phase Equilibria and Diffusion, 2018, 39, 584-591.	0.5	2
135	Interdiffusion and thermotransport in Niâ€“Al liquid alloys. Philosophical Magazine, 2018, 98, 2221-2246.	0.7	11
136	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.	0.3	8
137	A Thermodynamic Approach to Guide Reactive Element Doping: Hf Additions to NiCrAl. Oxidation of Metals, 2017, 87, 297-310.	1.0	11
138	Additive manufacturing of a functionally graded material from Ti-6Al-4V to Invar: Experimental characterization and thermodynamic calculations. Acta Materialia, 2017, 127, 133-142.	3.8	298
139	An improved sampling strategy for global energy minimization of multi-component systems. Computational Materials Science, 2017, 130, 282-291.	1.4	11
140	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
141	High strength Mg-Zn-Y alloys reinforced synergistically by Mg12ZnY phase and Mg3Zn3Y2 particle. Journal of Alloys and Compounds, 2017, 703, 508-516.	2.8	50
142	A physical model of thermal vacancies within the CALPHAD approach. Scripta Materialia, 2017, 133, 5-8.	2.6	12
143	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.	1.2	11
144	Tuning Phase Transitions in 1T-TaS₂ via the Substrate. Nano Letters, 2017, 17, 3471-3477.	4.5	55

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145	Compositional design of Fe-based multi-component bulk metallic glass based on CALPHAD method. Materials and Design, 2017, 126, 47-56.	3.3	8
146	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
147	High strength Mg 94 Zn 2.4 Y 3.6 alloy with long period stacking ordered structure prepared by near-rapid solidification technology. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2017, 679, 476-483.	2.6	18
148	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
149	High-Throughput Thermodynamic Modeling and Uncertainty Quantification for ICME. Jom, 2017, 69, 886-892.	0.9	31
150	Quantum behavior of water nano-confined in beryl. Journal of Chemical Physics, 2017, 146, 124307.	1.2	18
151	First-principles calculations and thermodynamic modeling of the Sn-Ta system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 57, 46-54.	0.7	4
152	Insight into the Mechanism of Thermal Stability of Î±-Diimine Nickel Complex in Catalyzing Ethylene Polymerization. Organometallics, 2017, 36, 1196-1203.	1.1	22
153	Phase equilibria, thermodynamics and microstructure simulation of metastable spinodal decomposition in câ€“Ti1â^'xAlxN coatings. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 56, 92-101.	0.7	33
154	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.	0.7	8
155	Zinc-induced embrittlement in nickel-base superalloys by simulation and experiment. Philosophical Magazine Letters, 2017, 97, 335-342.	0.5	3
156	Solute-induced solid-solution softening and hardening in bcc tungsten. Acta Materialia, 2017, 141, 304-316.	3.8	88
157	A curved pathway for oxygen interstitial diffusion in aluminum. Computational Materials Science, 2017, 140, 47-54.	1.4	10
158	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
159	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
160	Insight into Î³-Ni/Î³â€²-Ni3Al interfacial energy affected by alloying elements. Materials and Design, 2017, 133, 39-46.	3.3	39
161	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	1.4	223
162	First-principles calculations and thermodynamic modeling of the Yb-Ni binary system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 59, 207-217.	0.7	10

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