Zi-Kui Liu

List of Publications by Year in Descending Order

596 papers	20,266 citations	70 h-index	113 g-index
618 ext. papers	23,003 ext. citations	4.5 avg, IF	7.06 L-index

#	Paper	IF	Citations
596	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	6.1	1
595	Atomic control of active-site ensembles in ordered alloys to enhance hydrogenation selectivity.. *Nature Chemistry*, **2022**,	17.6	6
594	Predictive Crystal Plasticity Modeling of Single Crystal Nickel Based on First-Principles Calculations. *Jom*, **2022**, 74, 1423-1434	2.1	0
593	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
592	Extensible Structure-Informed Prediction of Formation Energy with improved accuracy and usability employing neural networks. *Computational Materials Science*, **2022**, 208, 111254	3.2	2
591	Theory of cross phenomena and their coefficients beyond Onsager theorem. *Materials Research Letters*, **2022**, 10, 393-439	7.4	2
590	Atomic-scale unveiling of strengthening in interstitial solid soluted Nb-rich TiAl alloys. *Journal of Alloys and Compounds*, **2022**, 917, 165484	5.7	0
589	Electrochemical recovery of Nd using liquid metals (Bi and Sn) in LiCl-KCl-NdCl3. *Electrochimica Acta* , **2022**, 425, 140655	6.7	3
588	Sensitivity estimation for calculated phase equilibria **2021**, 36, 140		1
587	Thermodynamic modeling of the Al-Co-Cr-Fe-Ni high entropy alloys supported by key experiments. *Journal of Alloys and Compounds*, **2021**, 897, 162722	5.7	1
586	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
585	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	1.9	0
584	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
583	Adsorption-controlled growth of Ga2O3 by suboxide molecular-beam epitaxy. *APL Materials*, **2021**, 9, 031101	5.7	11
582	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	5.3	11
581	Stability, Elastic and Electronic Properties of Ta2N by First-Principles Calculations. *Crystals*, **2021**, 11, 445	2.3	1
580	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	6.1	1

579	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
578	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
577	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	6	1
576	Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified L12 Ni3Al. *Jom*, **2021**, 73, 2285-2292	2.1	0
575	Elastic3rd: A tool for calculating third-order elastic constants from first-principles calculations. *Computer Physics Communications*, **2021**, 261, 107777	4.2	5
574	Integrating data mining and machine learning to discover high-strength ductile titanium alloys. *Acta Materialia*, **2021**, 202, 211-221	8.4	25
573	Underpinned exploration for magnetic structure, lattice dynamics, electronic properties, and disproportionation of yttrium nickelate. *AIP Advances*, **2021**, 11, 015028	1.5	0
572	Comment on "Thermodiffusion: The physico-chemical mechanics view" [J. Chem. Phys. 154, 024112 (2021)]. *Journal of Chemical Physics*, **2021**, 155, 087101	3.9	2
571	Understanding the surface adsorption and oxidation of cubic Cr0.5Al0.5N by first-principles calculations. *Computational Materials Science*, **2021**, 196, 110518	3.2	1
570	Revisiting the third-order elastic constants of diamond: The higher-order effect. *Diamond and Related Materials*, **2021**, 117, 108490	3.5	3
569	Tensile behavior of stainless steel 304L to Ni-20Cr functionally graded material: Experimental characterization and computational simulations. *Materialia*, **2021**, 18, 101151	3.2	3
568	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. *Acta Materialia*, **2021**, 217, 117169	8.4	6
567	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	5	3
566	Sensitivity estimation for calculated phase equilibria. *Journal of Materials Research*, **2021**, 36, 140-150	2.5	2
565	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	1	1
564	Exact phenomenological theory for thermotransport in a solid binary alloy. *Philosophical Magazine Letters*, **2021**, 101, 123-131	1	1
563	Forming mechanism of equilibrium and non-equilibrium metallurgical phases in dissimilar aluminum/steel (Al-Fe) joints.. *Scientific Reports*, **2021**, 11, 24251	4.9	1
562	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

561	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
560	Thermodynamic re-assessment of pure chromium using modified segmented regression model. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2020**, 69, 101762	1.9	4
559	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. *Engineering*, **2020**, 6, 612-620	9.7	1
558	View and Comments on the Data Ecosystem: Ocean of Data *Engineering*, **2020**, 6, 604-608	9.7	
557	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
556	Experimental phase diagram, thermodynamic modeling and solidified microstructure in the MoNiW ternary system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2020**, 68, 101748	1.9	6
555	Experimental validation of Scheil Gulliver simulations for gradient path planning in additively manufactured functionally graded materials. *Materialia*, **2020**, 11, 100689	3.2	17
554	Freestanding ultra-thin silica. *AIP Advances*, **2020**, 10, 025126	1.5	0
553	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
552	An orthorhombic D022-like precursor to Al8Mo3 in the AlMoTi system. *Journal of Alloys and Compounds*, **2020**, 823, 153807	5.7	4
551	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
550	Anomalous phonon-mode dependence in polarized Raman spectroscopy of the topological Weyl semimetal TaP. *Physical Review B*, **2020**, 101,	3.3	3
549	Anisotropic Fano resonance in the Weyl semimetal candidate LaAlSi. *Physical Review B*, **2020**, 102,	3.3	6
548	Thermodynamic Properties of Sr Sn Alloys via Emf Measurements and Thermal Analysis. *Journal of the Electrochemical Society*, **2020**, 167, 082508	3.9	3
547	Metastable trigonal SnP: A promising anode material for potassium-ion battery. *Carbon*, **2020**, 168, 468-474	10.4	19
546	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
545	Measurement of interdiffusivity for fcc_A1 Co-V-W alloys. *International Journal of Refractory Metals and Hard Materials*, **2020**, 87, 105134	4.1	2
544	Solute effects on the 111[11-0] tilt grain boundary in BCC Fe: Grain boundary segregation, stability, and embrittlement. *Computational Materials Science*, **2020**, 171, 109271	3.2	15

543	Computational thermodynamics and its applications. *Acta Materialia*, **2020**, 200, 745-792	8.4	36
542	Realization of Epitaxial Thin Films of the Topological Crystalline Insulator Sr SnO. *Advanced Materials*, **2020**, 32, e2000809	24	8
541	Experimental and computational studies of melting of the spinel phase in the Fe□Al□O ternary system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2020**, 70, 101798	1.9	0
540	Statistical approach for automated weighting of datasets: Application to heat capacity data. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2020**, 71, 101994	1.9	4
539	Suitability of binary oxides for molecular-beam epitaxy source materials: A comprehensive thermodynamic analysis. *APL Materials*, **2020**, 8, 081110	5.7	15
538	Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. *Computational Materials Science*, **2020**, 171, 109263	3.2	3
537	Diffusion of hydrogen isotopes in 3C-SiC in HTR-PM: A first-principles study. *Progress in Nuclear Energy*, **2020**, 119, 103181	2.3	0
536	Analysis of formation and growth of the □phase in additively manufactured functionally graded materials. *Journal of Alloys and Compounds*, **2020**, 814, 151729	5.7	18
535	Sintering mechanism of Cu-9Al alloy prepared from elemental powders. *Progress in Natural Science: Materials International*, **2019**, 29, 425-431	3.6	4
534	Local electronic descriptors for solute-defect interactions in bcc refractory metals. *Nature Communications*, **2019**, 10, 4484	17.4	11
533	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	4.4	9
532	Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys. *Acta Materialia*, **2019**, 181, 423-438	8.4	11
531	An alternative approach to predict Seebeck coefficients: Application to La3□Te4. *Scripta Materialia* , **2019**, 169, 87-91	5.6	7
530	Multiscale Entropy and Its Implications to Critical Phenomena, Emergent Behaviors, and Information. *Journal of Phase Equilibria and Diffusion*, **2019**, 40, 508-521	1	9
529	High-throughput thermodynamic calculations of phase equilibria in solidified 6016 Al-alloys. *Computational Materials Science*, **2019**, 167, 19-24	3.2	10
528	Multipoint Defect Synergy Realizing the Excellent Thermoelectric Performance of n-Type Polycrystalline SnSe via Re Doping. *Advanced Functional Materials*, **2019**, 29, 1902893	15.6	49
527	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
526	High Performance Anion Exchange Membrane Fuel Cells Enabled by Fluoropoly(olefin) Membranes. *Advanced Functional Materials*, **2019**, 29, 1902059	15.6	72

525	Quantified uncertainty in thermodynamic modeling for materials design. *Acta Materialia*, **2019**, 174, 9-15	8.4	21
524	Computer simulation of thermodynamic factors in Ni-Al and Cu-Ag liquid alloys. *Computational Materials Science*, **2019**, 166, 124-135	3.2	2
523	Local lattice distortion mediated formation of stacking faults in Mg alloys. *Acta Materialia*, **2019**, 170, 231-239	8.4	23
522	First-principles lattice dynamics and thermodynamic properties of pre-perovskite PbTiO3. *Acta Materialia*, **2019**, 171, 146-153	8.4	5
521	Experimental isothermal section of the Nb-Ni-Ru ternary system at 1100 °C. *Journal of Alloys and Compounds*, **2019**, 810, 151801	5.7	1
520	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
519	Atomic mobility evaluation and diffusion matrix for fcc_A1 Co□□W alloys. *Journal of Materials Science*, **2019**, 54, 13420-13432	4.3	4
518	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
517	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
516	ESPEI for efficient thermodynamic database development, modification, and uncertainty quantification: application to Cu□Mg. *MRS Communications*, **2019**, 9, 618-627	2.7	22
515	Phase equilibria of Ti□Al□ system at 1300 °C. *Intermetallics*, **2019**, 115, 106609	3.5	4
514	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
513	Application of Computational Thermodynamics for Magnesium Alloys Development **2019**, 311-335		
512	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
511	Mass and thermal transport in liquid Cu-Ag alloys. *Philosophical Magazine*, **2019**, 99, 468-491	1.6	8
510	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
509	Integrated computational materials engineering for advanced materials: A brief review. *Computational Materials Science*, **2019**, 158, 42-48	3.2	38
508	A piezoelectric, strain-controlled antiferromagnetic memory insensitive to magnetic fields. *Nature Nanotechnology*, **2019**, 14, 131-136	28.7	98

507	From random stacking faults to polytypes: A 12-layer NiSn4 polytype. *Journal of Alloys and Compounds*, **2019**, 774, 265-273	5.7	1
506	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
505	Synthesis science of SrRuO3 and CaRuO3 epitaxial films with high residual resistivity ratios. *APL Materials*, **2018**, 6, 046101	5.7	41
504	First-principles calculations of lattice dynamics and thermodynamic properties for Yb14MnSb11. *Journal of Applied Physics*, **2018**, 123, 045102	2.5	8
503	A quaternary sodium superionic conductor - Na10.8Sn1.9PS11.8. *Nano Energy*, **2018**, 47, 325-330	17.1	45
502	Martensitic transition in Fe via Bain path at finite temperatures: A comprehensive first-principles study. *Acta Materialia*, **2018**, 147, 261-276	8.4	18
501	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	5.7	48
500	Powder chemistry effects on the sintering of MgO-doped specialty Al2O3. *Journal of the American Ceramic Society*, **2018**, 101, 2739-2751	3.8	4
499	SnSe thin film solar cells produced by selenization of magnetron sputtered tin precursors. *Solar Energy Materials and Solar Cells*, **2018**, 176, 251-258	6.4	20
498	Accelerating exploitation of Co-Al-based superalloys from theoretical study. *Materials and Design*, **2018**, 142, 139-148	8.1	19
497	Electrically reversible cracks in an intermetallic film controlled by an electric field. *Nature Communications*, **2018**, 9, 41	17.4	42
496	Deposition of CVD-TiCN and TiAlN coatings guided with thermodynamic calculations. *International Journal of Materials Research*, **2018**, 109, 277-283	0.5	6
495	The Thermodynamic Database Database. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2018**, 61, 173-178	1.9	18
494	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	2.3	17
493	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
492	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
491	Phase stability and mechanical properties of AlHfNbTiZr high-entropy alloys. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2018**, 724, 249-259	5.3	36
490	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

489	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
488	Synergistic Effects of Nano-ZnO and Low pH of Sea Water on the Physiological Energetics of the Thick Shell Mussel. *Frontiers in Physiology*, **2018**, 9, 757	4.6	16
487	On Sluggish Diffusion in Fcc AlCoCrFeNi High-Entropy Alloys: An Experimental and Numerical Study. *Metals*, **2018**, 8, 16	2.3	44
486	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
485	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	1	1
484	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
483	Interdiffusion and thermotransport in NiAl liquid alloys. *Philosophical Magazine*, **2018**, 98, 2221-2246	1.6	7
482	High thermoelectric performance of few-quintuple Sb2Te3 nanofilms. *Nano Energy*, **2018**, 43, 285-290	17.1	38
481	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
480	Super-High Strength Mg97.5Al0.8Zn Alloy Prepared by Rapidly Solidified Powder Metallurgy and Low Temperature Extrusion. *Advanced Engineering Materials*, **2018**, 20, 1700712	3.5	1
479	Quasiharmonic calculations of thermodynamic properties for La3Te4 system. *Computational Materials Science*, **2018**, 142, 417-426	3.2	5
478	Design of Materials Processing Using Computational Thermodynamics **2018**, 27-45		
477	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	1.9	18
476	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
475	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
474	First-principles thermodynamic theory of Seebeck coefficients. *Physical Review B*, **2018**, 98,	3.3	17
473	Thermodynamic Assessment of the Ag-Se System Aided by First-Principles Calculations. *Journal of Phase Equilibria and Diffusion*, **2018**, 39, 870-881	1	1
472	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Mg3Sb2. *ACS Applied Energy Materials*, **2018**, 1, 6600-6608	6.1	17

471	Control of Epitaxial BaFeAs Atomic Configurations with Substrate Surface Terminations. *Nano Letters*, **2018**, 18, 6347-6352	11.5	11
470	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
469	Thermodynamic modeling of the La-Te system aided by first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2018**, 61, 227-236	1.9	4
468	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	2.5	12
467	Ocean of Data: Integrating First-Principles Calculations and CALPHAD Modeling with Machine Learning. *Journal of Phase Equilibria and Diffusion*, **2018**, 39, 635-649	1	19
466	A Thermodynamic Approach to Guide Reactive Element Doping: Hf Additions to NiCrAl. *Oxidation of Metals*, **2017**, 87, 297-310	1.6	10
465	Additive manufacturing of a functionally graded material from Ti-6Al-4V to Invar: Experimental characterization and thermodynamic calculations. *Acta Materialia*, **2017**, 127, 133-142	8.4	207
464	An improved sampling strategy for global energy minimization of multi-component systems. *Computational Materials Science*, **2017**, 130, 282-291	3.2	9
463	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
462	High strength Mg-Zn-Y alloys reinforced synergistically by Mg12ZnY phase and Mg3Zn3Y2 particle. *Journal of Alloys and Compounds*, **2017**, 703, 508-516	5.7	40
461	A physical model of thermal vacancies within the CALPHAD approach. *Scripta Materialia*, **2017**, 133, 5-8	5.6	10
460	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
459	Tuning Phase Transitions in 1T-TaS via the Substrate. *Nano Letters*, **2017**, 17, 3471-3477	11.5	40
458	Compositional design of Fe-based multi-component bulk metallic glass based on CALPHAD method. *Materials and Design*, **2017**, 126, 47-56	8.1	7
457	Origin of Outstanding Phase and Moisture Stability in a NaPAsS Superionic Conductor. *ACS Applied Materials & Interfaces*, **2017**, 9, 16261-16269	9.5	38
456	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	5.3	16
455	Revealing the Microstates of Body-Centered-Cubic (BCC) Equiatomic High Entropy Alloys. *Journal of Phase Equilibria and Diffusion*, **2017**, 38, 404-415	1	14
454	High-Throughput Thermodynamic Modeling and Uncertainty Quantification for ICME. *Jom*, **2017**, 69, 886-892	2.1	24

453	Quantum behavior of water nano-confined in beryl. *Journal of Chemical Physics*, **2017**, 146, 124307	3.9	16
452	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
451	Insight into the Mechanism of Thermal Stability of Diimine Nickel Complex in Catalyzing Ethylene Polymerization. *Organometallics*, **2017**, 36, 1196-1203	3.8	14
450	Phase equilibria, thermodynamics and microstructure simulation of metastable spinodal decomposition in c Ti1 AlxN coatings. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2017**, 56, 92-101	1.9	27
449	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
448	Zinc-induced embrittlement in nickel-base superalloys by simulation and experiment. *Philosophical Magazine Letters*, **2017**, 97, 335-342	1	2
447	Solute-induced solid-solution softening and hardening in bcc tungsten. *Acta Materialia*, **2017**, 141, 304-316	8.4	59
446	A curved pathway for oxygen interstitial diffusion in aluminum. *Computational Materials Science*, **2017**, 140, 47-54	3.2	8
445	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
444	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
443	Insight into Ni/ -Ni3Al interfacial energy affected by alloying elements. *Materials and Design*, **2017**, 133, 39-46	8.1	21
442	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. *Computational Materials Science*, **2017**, 139, 140-152	3.2	142
441	First-principles calculations and thermodynamic modeling of the Yb-Ni binary system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2017**, 59, 207-217	1.9	6
440	First-principles investigation of strain effects on the stacking fault energies, dislocation core structure, and Peierls stress of magnesium and its alloys. *Physical Review B*, **2017**, 95,	3.3	26
439	Atomic and electronic basis for the serrations of refractory high-entropy alloys. *Npj Computational Materials*, **2017**, 3,	10.9	39
438	Strengthening Mg by self-dispersed nano-lamellar faults. *Materials Research Letters*, **2017**, 5, 415-425	7.4	15
437	A lightweight single-phase AlTiVCr compositionally complex alloy. *Acta Materialia*, **2017**, 123, 115-124	8.4	97
436	Thermodynamic reassessment of the NiSiTi system using a four-sublattice model for ordered/disordered fcc phases supported by first-principles calculations. *Journal of Alloys and Compounds*, **2017**, 693, 344-356	5.7	10

435	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
434	Fundamentals of Thermal Expansion and Thermal Contraction. *Materials*, **2017**, 10,	3.5	9
433	Exploiting kinetics and thermodynamics to grow phase-pure complex oxides by molecular-beam epitaxy under continuous codeposition. *Physical Review Materials*, **2017**, 1,	3.2	16
432	Topological origin of the type-II Dirac fermions in PtSe2. *Physical Review Materials*, **2017**, 1,	3.2	30
431	A thermodynamic description of metastable c-TiAlZrN coatings with triple spinodally decomposed domains. *Journal of Mining and Metallurgy, Section B: Metallurgy*, **2017**, 53, 85-93	1	3
430	pycalphad: CALPHAD-based Computational Thermodynamics in Python. *Journal of Open Research Software*, **2017**, 5,	2.3	46
429	Adsorption-controlled growth of La-doped BaSnO3 by molecular-beam epitaxy. *APL Materials*, **2017**, 5, 116107	5.7	98
428	A hybrid functional study of native point defects in CuSnS: implications for reducing carrier recombination. *Physical Chemistry Chemical Physics*, **2017**, 20, 256-261	3.6	11
427	Lateral Versus Vertical Growth of Two-Dimensional Layered Transition-Metal Dichalcogenides: Thermodynamic Insight into MoS2. *Nano Letters*, **2016**, 16, 5742-50	11.5	70
426	Lattice dynamics, thermodynamics and elastic properties of C22-Zr6FeSn2 from first-principles calculations. *Journal of Nuclear Materials*, **2016**, 479, 461-469	3.3	8
425	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
424	Fabrication of nano-porous □Al2O3 layers on porous Ti-48Al-6Nb alloys. *Materials and Design*, **2016**, 109, 700-708	8.1	6
423	Stacking disorder in metastable NiSn4. *Materials and Design*, **2016**, 109, 324-333	8.1	7
422	First-principles calculations of lattice dynamics and thermal properties of polar solids. *Npj Computational Materials*, **2016**, 2,	10.9	88
421	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		
420	C15 NbCr2 Laves phase with mechanical properties beyond Pugh□ criterion. *Computational Materials Science*, **2016**, 121, 167-173	3.2	10
419	Thermodynamics of the S□n system: Implication for synthesis of earth abundant photovoltaic absorber materials. *Solar Energy*, **2016**, 125, 314-323	6.8	27
418	Thermodynamic modeling of Al□Co□r, Al□Co□Ni, Co□r□Ni ternary systems towards a description for Al□Co□r□Ni. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2016**, 52, 125-142	1.9	40

417	Synthesis, characterization and chemical stability of silicon dichalcogenides, Si(SexS1−x)2. *Journal of Crystal Growth*, **2016**, 452, 151-157	1.6	10
416	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
415	Functionally graded material of 304L stainless steel and inconel 625 fabricated by directed energy deposition: Characterization and thermodynamic modeling. *Acta Materialia*, **2016**, 108, 46-54	8.4	266
414	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
413	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
412	Diffusion coefficients of alloying elements in dilute Mg alloys: A comprehensive first-principles study. *Acta Materialia*, **2016**, 103, 573-586	8.4	108
411	New Phases in Mg-Al-Ca System **2016**, 427-432		1
410	Computational Thermodynamics of Materials **2016**,		28
409	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		
408	Computational Thermodynamics and Experimental Investigation of the Mg-Al-Ca-Sr Alloys **2016**, 421-425		
407	Computational Thermodynamics and Experimental Investigation of Mg-Al-Ca Alloys **2016**, 415-419		
406	First-principles Study of Diffusion Coefficients of Alloy Elements in Dilute Mg Alloys **2016**, 97-101		
405	Design Magnesium Alloys: How Computational Thermodynamics Can Help **2016**, 403-410		
404	Thermodynamic remodeling of the Al–Pt system towards an assessment of the Al–Ni–Pt system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2016**, 55, 88-102	1.9	3
403	On the mean kinetic energy of the proton in strong hydrogen bonded systems. *Journal of Chemical Physics*, **2016**, 144, 054302	3.9	11
402	Abnormal correlation between phase transformation and cooling rate for pure metals. *Scientific Reports*, **2016**, 6, 22391	4.9	17
401	Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias. *Advanced Materials*, **2016**, 28, 118-23	24	18
400	Ferromagnetism: Epitaxial Growth of Intermetallic MnPt Films on Oxides and Large Exchange Bias (Adv. Mater. 1/2016). *Advanced Materials*, **2016**, 28, 204-204	24	

399	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
398	Generalization of first-principles thermodynamic model: Application to hexagonal close-packed Fe3N. *Computational Materials Science*, **2016**, 117, 83-89	3.2	4
397	Power law scaled hardness of Mn strengthened nanocrystalline Al Mn non-equilibrium solid solutions. *Scripta Materialia*, **2016**, 120, 31-36	5.6	17
396	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
395	First-principles Study of Diffusion Coefficients of Alloy Elements in Dilute Mg Alloys **2016**, 97-101		
394	Influence of the interatomic potential on thermotransport in binary liquid alloys: case study on NiAl. *Philosophical Magazine*, **2016**, 96, 3054-3074	1.6	11
393	Phase transformation in Ti48Al8Nb porous alloys and its influence on pore properties. *Materials and Design*, **2015**, 83, 508-513	8.1	17
392	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
391	Ti-substituted Li[Li0.26Mn0.6TixNi0.07Co0.07]O2 layered cathode material with improved structural stability and suppressed voltage fading. *Journal of Materials Chemistry A*, **2015**, 3, 17376-17384	13	33
390	A novel hot pack rolling of high NbTiAl sheet from cast ingot. *Intermetallics*, **2015**, 67, 19-25	3.5	33
389	Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study. *Acta Materialia*, **2015**, 97, 75-85	8.4	46
388	Nano-sized Superlattice Clusters Created by Oxygen Ordering in Mechanically Alloyed Fe Alloys. *Scientific Reports*, **2015**, 5, 11772	4.9	10
387	Rebuttal comments on Mitigating grain growth in binary nanocrystalline alloys through solute selection based on thermodynamic stability maps *Computational Materials Science*, **2015**, 107, 238-242	3.2	1
386	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
385	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
384	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
383	Bonding charge density from atomic perturbations. *Journal of Computational Chemistry*, **2015**, 36, 1008-14	3.5	15
382	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

381	Strain-induced dimensionality crossover of precursor modulations in Ni2MnGa. *Applied Physics Letters*, **2015**, 106, 021910	3.4	3
380	Cr-based bulk metallic glasses with ultrahigh hardness. *Applied Physics Letters*, **2015**, 106, 251905	3.4	17
379	A thermodynamic re-assessment of Al□V toward an assessment of the ternary Al□Ti□V system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2015**, 51, 75-88	1.9	21
378	Thermodynamic modeling of the aluminum□iron□oxygen system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2015**, 51, 178-192	1.9	10
377	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
376	An integrated fast Fourier transform-based phase-field and crystal plasticity approach to model recrystallization of three dimensional polycrystals. *Computer Methods in Applied Mechanics and Engineering*, **2015**, 285, 829-848	5.7	79
375	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
374	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
373	Molecular dynamics simulations of the effects of vacancies on nickel self-diffusion, oxygen diffusion and oxidation initiation in nickel, using the ReaxFF reactive force field. *Acta Materialia*, **2015**, 83, 102-112	8.4	65
372	Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. *Acta Materialia*, **2015**, 82, 287-294	8.4	23
371	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
370	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
369	Experimental study and thermodynamic modeling of the Al-Co-Cr-Ni system. *Science and Technology of Advanced Materials*, **2015**, 16, 055001	7.1	16
368	Atomic-Level Mechanisms of Nucleation of Pure Liquid Metals during Rapid Cooling. *ChemPhysChem*, **2015**, 16, 3916-27	3.2	11
367	First-principles calculations, experimental study, and thermodynamic modeling of the Al-Co-Cr system. *PLoS ONE*, **2015**, 10, e0121386	3.7	11
366	Nb□Al diffusion reaction in high Nb containing TiAl porous alloys. *Materials Science and Technology*, **2015**, 31, 1388-1391	1.5	8
365	A Fundamental Stability Study for Amorphous LiLaTiO3Solid Electrolyte. *Journal of the Electrochemical Society*, **2015**, 162, A244-A248	3.9	38
364	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

363	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
362	Alloying effects of Ta on the mechanical properties of □Co3(Al, W): A first-principles study. *Scripta Materialia*, **2015**, 100, 5-8	5.6	20
361	C-vacancy concentration in cementite, Fe3C1□in equilibrium with □Fe[C] and □Fe[C]. *Acta Materialia*, **2015**, 86, 374-384	8.4	16
360	Nature of ferroelectric-paraelectric phase transition and origin of negative thermal expansion in PbTiO3. *Physical Review B*, **2015**, 91,	3.3	25
359	Thermal expansion anomaly regulated by entropy. *Scientific Reports*, **2014**, 4, 7043	4.9	46
358	Developing gradient metal alloys through radial deposition additive manufacturing. *Scientific Reports*, **2014**, 4, 5357	4.9	154
357	Vacancy mechanism of oxygen diffusivity in bcc Fe: A first-principles study. *Corrosion Science*, **2014**, 83, 94-102	6.8	47
356	Temperature-dependent mechanical properties of alpha-/beta-Nb5Si3 phases from first-principles calculations. *Intermetallics*, **2014**, 46, 72-79	3.5	26
355	A first-principles study of self-diffusion coefficients of fcc Ni. *Computational Materials Science*, **2014** , 86, 17-23	3.2	27
354	Amorphous LiLaTiO3as Solid Electrolyte Material. *Journal of the Electrochemical Society*, **2014**, 161, A473-A479	3.9	29
353	Reaction behavior and pore formation mechanism of TiAl□Nb porous alloys prepared by elemental powder metallurgy. *Intermetallics*, **2014**, 44, 1-7	3.5	32
352	Mitigating grain growth in binary nanocrystalline alloys through solute selection based on thermodynamic stability maps. *Computational Materials Science*, **2014**, 84, 255-266	3.2	94
351	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
350	Sluggish mobility and strong icosahedral ordering in Mg□Zn□Ca liquid and glassy alloys. *Acta Materialia*, **2014**, 67, 266-277	8.4	15
349	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
348	First-principles study of the mechanical properties and phase stability of TiO2. *Computational Materials Science*, **2014**, 83, 114-119	3.2	26
347	Origin of enhanced glass-forming ability of Ce-containing Al□e alloy: Ab initio molecular dynamics study. *Intermetallics*, **2014**, 46, 29-39	3.5	10
346	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

345	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
344	Effect of solute atoms on glass-forming ability for Fe□B alloy: An ab initio molecular dynamics study. *Acta Materialia*, **2014**, 77, 96-110	8.4	21
343	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
342	First-principles calculations and thermodynamic modeling of the Sn□r and Mg□n□r systems. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 46, 237-248	1.9	16
341	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
340	Perspective on Materials Genome□ . *Science Bulletin*, **2014**, 59, 1619-1623		26
339	Toward an integrated computational system for describing the additive manufacturing process for metallic materials. *Additive Manufacturing*, **2014**, 1-4, 52-63	6.1	54
338	YPHON: A package for calculating phonons of polar materials. *Computer Physics Communications*, **2014**, 185, 2950-2968	4.2	35
337	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
336	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
335	Glass formability of W-based alloys through thermodynamic modeling: W□e□f□d□a and W□e□i□. *Intermetallics*, **2014**, 48, 79-85	3.5	6
334	Structure and energetics of Ni from ab initio molecular dynamics calculations. *Computational Materials Science*, **2014**, 89, 242-246	3.2	10
333	Quantifying charge ordering by density functional theory: Fe3O4 and CaFeO3. *Chemical Physics Letters*, **2014**, 607, 81-84	2.5	10
332	Thermotransport in binary system: case study on Ni50Al50 melt. *Philosophical Magazine*, **2014**, 94, 3574-3602	1.6	17
331	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
330	Toward Metamodels for Composable and Reusable Additive Manufacturing Process Models. *Journal of Manufacturing Science and Engineering, Transactions of the ASME*, **2014**, 136,	3.3	37
329	Mo-doped TiO2 with enhanced visible light photocatalytic activity: a combined experimental and theoretical study. *Journal of Nanoscience and Nanotechnology*, **2014**, 14, 6865-71	1.3	37
328	The development of phase-based property data using the CALPHAD method and infrastructure needs. *Integrating Materials and Manufacturing Innovation*, **2014**, 3, 158-180	2.9	26

327	Compositionally graded metals: A new frontier of additive manufacturing. *Journal of Materials Research*, **2014**, 29, 1899-1910	2.5	129
326	The Penn State-Georgia Tech CCMD: ushering in the ICME Era. *Integrating Materials and Manufacturing Innovation*, **2014**, 3, 409-428	2.9	5
325	Solution-based thermodynamic modeling of the Ni-Al-Mo system using first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2014**, 46, 124-133	1.9	15
324	File and data repositories for Next Generation CALPHAD. *Scripta Materialia*, **2014**, 70, 7-11	5.6	28
323	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
322	Efficient stochastic generation of special quasirandom structures. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2013**, 42, 13-18	1.9	572
321	Ab initio molecular dynamics simulation of the liquid and amorphous structure of Mg65Cu25Gd10 alloy. *Physica B: Condensed Matter*, **2013**, 426, 65-70	2.8	3
320	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	
319	Accurate determination of thermodynamic properties for liquid alloys based on ab initio molecular dynamics simulation. *Fluid Phase Equilibria*, **2013**, 360, 44-53	2.5	9
318	Density Functional Theory-Based Database Development and CALPHAD Automation. *Jom*, **2013**, 65, 1533-1539	2.1	13
317	Thermodynamic properties of magnesium alloys **2013**, 85-124		
316	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
315	Experimental and computational studies of the Cu-Hf binary system. *Acta Materialia*, **2013**, 61, 660-669	8.4	4
314	First-principles aided thermodynamic modeling of the Nb-Re system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2013**, 41, 119-127	1.9	15
313	First-principles investigation of electronic, mechanical and thermodynamic properties of L12 ordered Co3(M, W) (M = Al, Ge, Ga) phases. *Acta Materialia*, **2013**, 61, 5437-5448	8.4	59
312	BiFeO3 domain wall energies and structures: a combined experimental and density functional theory+U study. *Physical Review Letters*, **2013**, 110, 267601	7.4	49
311	Structural mechanism for ultrahigh-strength Co-based metallic glasses. *Scripta Materialia*, **2013**, 68, 257-260	3.6	11
310	Accurate calculations of phonon dispersion in CaF2 and CeO2. *Physical Review B*, **2013**, 88,	3.3	21

309	Low energy structures of lithium-ion battery materials Li(MnxNixCo1−2x)O2 revealed by first-principles calculations. *Applied Physics Letters*, **2013**, 103, 053903	3.4	9
308	Defect Chemistry and Phase Equilibria of (La1-xCax)FeO3-δ: Thermodynamic Modeling. *Journal of the Electrochemical Society*, **2013**, 160, F1103-F1108	3.9	17
307	Computational Thermodynamics and Experimental Investigation of Mg-Al-Ca Alloys **2013**, 113-117		2
306	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
305	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
304	Electron localization morphology of the stacking faults in Mg: A first-principles study. *Chemical Physics Letters*, **2012**, 551, 121-125	2.5	29
303	Mixed-space approach for calculation of vibration-induced dipole-dipole interactions. *Physical Review B*, **2012**, 85,	3.3	33
302	Effects of reactive elements on the structure and diffusivity of liquid chromia: An ab initio molecular dynamics study. *Physical Review B*, **2012**, 85,	3.3	18
301	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
300	First-principles lattice dynamics, thermodynamics, and elasticity of Cr2O3. *Surface Science*, **2012**, 606, 1422-1425	1.8	42
299	Maximizing the number of coexisting phases near invariant critical points for giant electrocaloric and electromechanical responses in ferroelectrics. *Applied Physics Letters*, **2012**, 101, 082904	3.4	67
298	Fabrication and characterization of beaded SiC quantum rings with anomalous red spectral shift. *Advanced Materials*, **2012**, 24, 5598-603	24	59
297	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. *Acta Materialia*, **2012**, 60, 5204-5216	8.4	58
296	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
295	Thermodynamic properties of Laves phases in the Mg-Al-Ca system at finite temperature from first-principles. *Intermetallics*, **2012**, 22, 17-23	3.5	23
294	Thermodynamic and mechanical properties of lanthanum–magnesium phases from density functional theory. *Journal of Alloys and Compounds*, **2012**, 512, 296-310	5.7	56
293	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
292	The adsorption-controlled growth of LuFe2O4 by molecular-beam epitaxy. *Applied Physics Letters*, **2012**, 101, 132907	3.4	32

291	Defects in boron carbide: First-principles calculations and CALPHAD modeling. *Acta Materialia*, **2012**, 60, 7207-7215	8.4	11
290	First-principles calculations and thermodynamic re-modeling of the HfN system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2012**, 38, 92-99	1.9	15
289	Phase stability and thermodynamic modeling of the ReTi system supplemented by first-principles calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2012**, 38, 71-80	1.9	11
288	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
287	Effects of Alloying Elements on Elastic, Stacking Fault, and Diffusion Properties of Fcc Ni from First-Principles: Implications for Tailoring the Creep Rate of Ni-Base Superalloys **2012**, 455-461		8
286	Foreword: Hume-Rothery Symposium on Thermodynamics and Diffusion Coupling in Alloys—Application Driven Science. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2012**, 43, 3452-3452	2.3	
285	First-principles calculations of interfacial and segregation energies in Cr2O3. *Journal of Physics Condensed Matter*, **2012**, 24, 225001	1.8	6
284	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
283	A first-principles approach to transition states of diffusion. *Journal of Physics Condensed Matter*, **2012**, 24, 305402	1.8	8
282	Effects of alloying elements and temperature on the elastic properties of dilute Ni-base superalloys from first-principles calculations. *Journal of Applied Physics*, **2012**, 112, 053515	2.5	59
281	Nature of ferroelectric–paraelectric transition. *Philosophical Magazine Letters*, **2012**, 92, 399-407	1	11
280	Effects of alloying elements on thermal expansions of γ-Ni and γ′-Ni3Al by first-principles calculations. *Acta Materialia*, **2012**, 60, 1846-1856	8.4	28
279	Phase-field simulations of thickness-dependent domain stability in PbTiO3 thin films. *Acta Materialia*, **2012**, 60, 3296-3301	8.4	15
278	First-principles calculation of structural, mechanical, magnetic and thermodynamic properties for M23C6 (M = Fe, Cr) compounds. *Journal of Physics Condensed Matter*, **2012**, 24, 505503	1.8	27
277	Crystal structure determination of Hägg carbide, Fe5C2 by first-principles calculations and Rietveld refinement. *Zeitschrift Für Kristallographie*, **2012**, 227, 207-220		21
276	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
275	Phonon and thermodynamic properties of AlMn compounds: A first-principles study. *Computational Materials Science*, **2011**, 50, 2096-2103	3.2	16
274	First-principles calculations and thermodynamic modeling of the AlPt binary system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2011**, 35, 20-29	1.9	31

273	Experimental investigation and thermodynamic modeling of the CuSiZn system with the refined description for the CuZn system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2011**, 35, 191-203	1.9	9
272	Thermodynamic modeling of fcc order/disorder transformations in the CoPt system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2011**, 35, 323-330	1.9	20
271	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
270	Anomalous energy pathway of vacancy migration and self-diffusion in hcp Ti. *Physical Review B*, **2011**, 83,	3.3	34
269	Hybrid Functionals Study of Band Bowing, Band Edges and Electronic Structures of Cd1−xZnxS Solid Solution. *Journal of Physical Chemistry C*, **2011**, 115, 19741-19748	3.8	78
268	First-principles calculations of phonon and thermodynamic properties of Fe-Si compounds. *Intermetallics*, **2011**, 19, 1374-1384	3.5	31
267	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
266	Effect of Lead Oxide Vapor on the Strength of Alumina. *International Journal of Applied Ceramic Technology*, **2011**, 8, 1517-1524	2	4
265	Origin of negative thermal expansion phenomenon in solids. *Scripta Materialia*, **2011**, 65, 664-667	5.6	32
264	Effect of carbon on lattice parameters of the MgB2 thin films: A computational study. *Physica C: Superconductivity and Its Applications*, **2011**, 471, 553-557	1.3	
263	Elastic properties of cubic, tetragonal and monoclinic ZrO2 from first-principles calculations. *Journal of Nuclear Materials*, **2011**, 415, 13-17	3.3	61
262	Magnetic excitation and thermodynamics of BaFe2As2. *International Journal of Quantum Chemistry*, **2011**, 111, 3565-3570	2.1	5
261	First-principles study of lattice dynamics and thermodynamics of TiO2 polymorphs. *Inorganic Chemistry*, **2011**, 50, 6996-7003	5.1	57
260	First-principles calculations of impurity diffusion coefficients in dilute Mg alloys using the 8-frequency model. *Acta Materialia*, **2011**, 59, 3214-3228	8.4	112
259	First-principles lattice dynamics and heat capacity of BiFeO3. *Acta Materialia*, **2011**, 59, 4229-4234	8.4	46
258	Atomic structure and diffusivity in liquid Al80Ni20 by ab initio molecular dynamics simulations. *Physica B: Condensed Matter*, **2011**, 406, 3089-3097	2.8	37
257	Effects of spin structures on Fermi surface topologies in BaFe2As2. *Solid State Communications*, **2011**, 151, 272-275	1.6	3
256	Structural, vibrational, and thermodynamic properties of ordered and disordered Ni1−xPtx alloys from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	42

255	Thermodynamics of multiferroic BiFeO3: Applications for the deposition of BiFeO3 thin films. *Applied Physics Letters*, **2011**, 98, 131904	3.4	10
254	Native defects in LiNH2: A first-principles study. *Physical Review B*, **2011**, 84,	3.3	16
253	First-Principles Thermochemistry and Thermodynamic Modeling of the Al2O3Nd2O3SiO2Y2O3 Pseudoquaternary System. *Journal of the American Ceramic Society*, **2010**, 93, 4158-4167	3.8	11
252	Thermodynamic fluctuations in magnetic states: Fe3Pt as a prototype. *Philosophical Magazine Letters*, **2010**, 90, 851-859	1	29
251	Adsorption-controlled growth of BiMnO3 films by molecular-beam epitaxy. *Applied Physics Letters*, **2010**, 96, 262905	3.4	35
250	Effects of spin structures on phonons in BaFe2As2. *Applied Physics Letters*, **2010**, 97, 022504	3.4	3
249	Phase transitions and domain stabilities in biaxially strained (001) SrTiO3 epitaxial thin films. *Journal of Applied Physics*, **2010**, 108, 084113	2.5	20
248	Thermodynamic fluctuations between magnetic states from first-principles phonon calculations: The case of bcc Fe. *Physical Review B*, **2010**, 82,	3.3	33
247	Phonon dispersion in Sr2RuO4 studied by a first-principles cumulative force-constant approach. *Physical Review B*, **2010**, 82,	3.3	13
246	A modified Landau□Devonshire thermodynamic potential for strontium titanate. *Applied Physics Letters*, **2010**, 96, 232902	3.4	31
245	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
244	Magnetic perturbation and associated energies of the antiphase boundaries in ordered Ni3Al. *Journal of Applied Physics*, **2010**, 108, 103509	2.5	21
243	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
242	First-principles study of structural and elastic properties of monoclinic and orthorhombic BiMnO3. *Journal of Physics Condensed Matter*, **2010**, 22, 295404	1.8	7
241	A first-principles scheme to phonons of high temperature phase: No imaginary modes for cubic SrTiO3. *Applied Physics Letters*, **2010**, 97, 162907	3.4	8
240	Temperature-dependent elastic stiffness constants of □and □Al2O3 from first-principles calculations. *Journal of Physics Condensed Matter*, **2010**, 22, 375403	1.8	54
239	Thermodynamic properties of Co3O4 and Sr6Co5O15 from first-principles. *Inorganic Chemistry*, **2010**, 49, 10291-8	5.1	14
238	Structural and thermodynamic properties of compounds in the MgB□ system from first-principles calculations. *Intermetallics*, **2010**, 18, 803-808	3.5	9

237	Entropy favored ordering: Phase stability of Ni3Pt revisited by first-principles. *Intermetallics*, **2010**, 18, 961-964	3.5	23
236	Effects of alloying elements on elastic properties of Ni3Al by first-principles calculations. *Intermetallics*, **2010**, 18, 1163-1171	3.5	71
235	First-principles calculations and thermodynamic modeling of the Re-Y system with extension to the Ni-Re-Y system. *Intermetallics*, **2010**, 18, 2412-2418	3.5	10
234	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
233	Solvus boundaries of (meta)stable phases in the Al-Mg-Si system: First-principles phonon calculations and thermodynamic modeling. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2010**, 34, 20-25	1.9	23
232	First-principles calculations and thermodynamic modeling of Cs-I system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2010**, 34, 134-137	1.9	2
231	First-principles thermodynamics from phonon and Debye model: Application to Ni and Ni3Al. *Computational Materials Science*, **2010**, 47, 1040-1048	3.2	278
230	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
229	First-principles calculations of pure elements: Equations of state and elastic stiffness constants. *Computational Materials Science*, **2010**, 48, 813-826	3.2	219
228	First-principles study of self-diffusion in hcp Mg and Zn. *Computational Materials Science*, **2010**, 50, 301-307	3.2	55
227	Magnetic thermodynamics of fcc Ni from first-principles partition function approach. *Journal of Applied Physics*, **2010**, 108, 123514	2.5	25
226	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
225	A first-principles approach to finite temperature elastic constants. *Journal of Physics Condensed Matter*, **2010**, 22, 225404	1.8	136
224	Ab initio molecular dynamics simulation of the atom packing and density of Al-Ni amorphous alloys. *Science China Technological Sciences*, **2010**, 53, 3175-3182	3.5	11
223	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
222	Phase Stability and Oxidation Behavior of an Alumina Scale-Forming NiCrAlY Alloy. *Oxidation of Metals*, **2010**, 74, 179-191	1.6	5
221	First-principles calculations of twin-boundary and stacking-fault energies in magnesium. *Scripta Materialia*, **2010**, 62, 646-649	5.6	123
220	Computational modeling of effects of alloying elements on elastic coefficients. *Scripta Materialia*, **2010**, 63, 686-691	5.6	35

219	High-zirconium-based bulk metallic glasses with large plasticity. *Scripta Materialia*, **2010**, 63, 239-242	5.6	40
218	Effect of Mg, Ca, and Zn on stability of LiBH4 through computational thermodynamics. *International Journal of Hydrogen Energy*, **2010**, 35, 6812-6821	6.7	23
217	First-principles calculations of the elastic, phonon and thermodynamic properties of Al12Mg17. *Acta Materialia*, **2010**, 58, 4012-4018	8.4	81
216	Coarsening Kinetics of a Two Phase Mixture with Highly Disparate Diffusion Mobility. *Communications in Computational Physics*, **2010**, 8, 249-264	2.4	30
215	3d transition metal impurities in aluminum: A first-principles study. *Physical Review B*, **2009**, 80,	3.3	53
214	Diffusion of hydrogen vacancy in Na3AlH6. *Applied Physics Letters*, **2009**, 95, 111910	3.4	10
213	Density-functional study of the pressure-induced phase transitions in Ti at zero Kelvin. *Physical Review B*, **2009**, 79,	3.3	31
212	Intrinsic ferroelectric properties of the nonstoichiometric perovskite oxide Ba1−xTi1−yO3−2y. *Journal of Applied Physics*, **2009**, 105, 093519	2.5	27
211	Predicting Diffusion Coefficients from First Principles via Eyring's Reaction Rate Theory. *Defect and Diffusion Forum*, **2009**, 294, 1-13	0.7	22
210	A thermodynamic framework for a system with itinerant-electron magnetism. *Journal of Physics Condensed Matter*, **2009**, 21, 326003	1.8	23
209	Determination of phases in the system chromium–platinum (Cr–Pt) and thermodynamic calculations. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2009**, 510-511, 322-327	5.3	9
208	Thermodynamic calculations and phase diagrams for magnesium and its alloys: Part II. *Jom*, **2009**, 61, 67-67	2.1	
207	The EMPMD: A positive force in TMS programming. *Jom*, **2009**, 61, 10-10	2.1	1
206	A materials research paradigm driven by computation. *Jom*, **2009**, 61, 18-20	2.1	11
205	First-Principles Calculations and CALPHAD Modeling of Thermodynamics. *Journal of Phase Equilibria and Diffusion*, **2009**, 30, 517-534	1	243
204	Factors Limiting Equilibrium in Fabricating a Simple Ferroelectric Oxide: BaTiO3. *Journal of the American Ceramic Society*, **2009**, 92, 222-228	3.8	12
203	Endogenous ethanolamide analysis in human plasma using HPLC tandem MS with electrospray ionization. *Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences*, **2009**, 877, 2052-60	3.2	35
202	Atomic structure of Zr41.2Ti13.8Cu12.5Ni10Be22.5 bulk metallic glass alloy. *Acta Materialia*, **2009**, 57, 376-391	8.4	93

201	Effect of alloying elements on the elastic properties of Mg from first-principles calculations. *Acta Materialia*, **2009**, 57, 3876-3884	8.4	137
200	First principles impurity diffusion coefficients. *Acta Materialia*, **2009**, 57, 4102-4108	8.4	184
199	Al-centered icosahedral ordering in Cu46Zr46Al8 bulk metallic glass. *Applied Physics Letters*, **2009**, 94, 091904	3.4	56
198	Density-functional study of the thermodynamic properties and the pressure–temperature phase diagram of Ti. *Physical Review B*, **2009**, 80,	3.3	79
197	Predictions of the Al-rich region of the Al–Co–Ni–Y system based upon first-principles and experimental data. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 124-135	1.9	11
196	Thermodynamic investigation of the galvanizing systems, I: Refinement of the thermodynamic description for the Fe–Zn system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 433-440	1.9	34
195	Solution-based thermodynamic modeling of the Ni–Ta and Ni–Mo–Ta systems using first-principle calculations. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 631-641	1.9	29
194	Thermodynamic modeling of the Si–Sr system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2009**, 33, 550-556	1.9	9
193	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
192	Effects of alloying elements on elastic properties of Ni by first-principles calculations. *Computational Materials Science*, **2009**, 47, 254-260	3.2	66
191	Elastic constants of binary Mg compounds from first-principles calculations. *Intermetallics*, **2009**, 17, 313-318	3.5	168
190	Enthalpies of formation of magnesium compounds from first-principles calculations. *Intermetallics*, **2009**, 17, 878-885	3.5	131
189	Elastic properties of cubic and rhombohedral BiFeO3 from first-principles calculations. *Physical Review B*, **2009**, 80,	3.3	97
188	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
187	Adsorption-controlled growth of BiFeO3 by MBE and integration with wide band gap semiconductors. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **2009**, 56, 1528-33	3.2	14
186	Extreme elastic anisotropy of cementite, Fe3C: First-principles calculations and experimental evidence. *Scripta Materialia*, **2008**, 59, 814-817	5.6	72
185	First-principles calculation of self-diffusion coefficients. *Physical Review Letters*, **2008**, 100, 215901	7.4	197
184	Thermodynamic modeling of the Cu–Mn system supported by key experiments. *Journal of Alloys and Compounds*, **2008**, 457, 233-238	5.7	24

183	First-principles study of AlNiY ternary compounds for crystal structure validation. *Journal of Alloys and Compounds*, **2008**, 462, 262-266	5.7	11
182	Thermodynamic modeling of MgCaCe system by combining first-principles and CALPHAD method. *Journal of Alloys and Compounds*, **2008**, 463, 294-301	5.7	15
181	Prediction of the glass forming ability in CuZr binary and CuZrTi ternary alloys. *Intermetallics*, **2008**, 16, 27-33	3.5	29
180	Phase equilibria, thermodynamics and solidification microstructures of MgSnCa alloys, Part 1: Experimental investigation and thermodynamic modeling of the ternary MgSnCa system. *Intermetallics*, **2008**, 16, 299-315	3.5	76
179	Enthalpy of mixing for ternary fcc solid solutions from special quasirandom structures. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2008**, 32, 74-81	1.9	16
178	Summary of the CALPHAD XXXVI 2007 conference. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2008**, 32, 9-31	1.9	2
177	Thermodynamic modeling of the CuSi system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2008**, 32, 520-526	1.9	30
176	Readily regenerable reduced microstructure representations. *Computational Materials Science*, **2008**, 42, 368-379	3.2	1
175	Ab initio molecular dynamics simulation for structural transition of Zr during rapid quenching processes. *Computational Materials Science*, **2008**, 43, 1123-1129	3.2	31
174	Structural characterization of Mg65Cu25Y10 metallic glass from ab initio molecular dynamics. *Computational Materials Science*, **2008**, 44, 802-806	3.2	28
173	Misfit strainMisfit strain diagram of epitaxial BaTiO3 thin films: Thermodynamic calculations and phase-field simulations. *Applied Physics Letters*, **2008**, 93, 232904	3.4	44
172	Fully band-resolved scattering rate in MgB2 revealed by the nonlinear hall effect and magnetoresistance measurements. *Physical Review Letters*, **2008**, 101, 067001	7.4	53
171	Domain stability of PbTiO3 thin films under anisotropic misfit strains: Phase-field simulations. *Journal of Applied Physics*, **2008**, 104, 054105	2.5	34
170	Study of MgB2IPb tunnel junctions on MgO (211) substrates. *Applied Physics Letters*, **2008**, 93, 012502	3.4	22
169	Icosahedral ordering in Zr41Ti14Cu12.5Ni10Be22.5 bulk metallic glass. *Applied Physics Letters*, **2008**, 92, 201913	3.4	31
168	Optical band gap of BiFeO3 grown by molecular-beam epitaxy. *Applied Physics Letters*, **2008**, 92, 142908	3.4	300
167	Thermodynamics of the Ce Etransition: Density-functional study. *Physical Review B*, **2008**, 78,	3.3	69
166	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

165	Atomic structures of Zr-based metallic glasses **2008**, 51, 400-413		16
164	Thermodynamic calculations and phase diagrams for magnesium and its alloys: Part I. *Jom*, **2008**, 60, 31-31	2.1	7
163	The development and application of a thermodynamic database for magnesium alloys. *Jom*, **2008**, 60, 45-47	2.1	67
162	Thermodynamic Modeling of the Succinonitrile-Water System. *Journal of Phase Equilibria and Diffusion*, **2008**, 29, 247-251	1	6
161	Structural evolution of Cu during rapid quenching by ab initio molecular dynamics. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 5831-5837	2.3	26
160	The influence of interstitial distribution on phase stability and properties of hexagonal Fe6Cx, Fe6Ny and Fe6CxNy phases: A first-principles calculation. *Acta Materialia*, **2008**, 56, 719-725	8.4	21
159	Coarsening kinetics of precipitates in the NiAlMo system. *Acta Materialia*, **2008**, 56, 5544-5551	8.4	86
158	A thermodynamic description of the AlFeSi system over the whole composition and temperature ranges via a hybrid approach of CALPHAD and key experiments. *Intermetallics*, **2008**, 16, 554-570	3.5	149
157	Comprehensive Linkage of Defect and Phase Equilibria through Ferroelectric Transition Behavior in BaTiO3-Based Dielectrics: Part 1. Defect Energies Under Ambient Air Conditions. *Journal of the American Ceramic Society*, **2008**, 91, 1748-1752	3.8	23
156	Comprehensive Linkage of Defect and Phase Equilibria Through Ferroelectric Transition Behavior in BaTiO3-Based Dielectrics: Part 2. Defect Modeling Under Low Oxygen Partial Pressure Conditions. *Journal of the American Ceramic Society*, **2008**, 91, 1753-1761	3.8	27
155	First-Principles Calculations and Thermodynamic Modeling of the Al2O3Nd2O3 System. *Journal of the American Ceramic Society*, **2008**, 91, 3355-3361	3.8	11
154	Influence of nonstoichiometry on ferroelectric phase transition in BaTiO3. *Journal of Applied Physics*, **2007**, 101, 054119	2.5	65
153	Reassessment of the AlMn system and a thermodynamic description of the AlMgMn system. *International Journal of Materials Research*, **2007**, 98, 855-871	0.5	92
152	Integration of first-principles calculations, calphad modeling, and phase-field simulations **2007**, 171-213		3
151	Prediction of the Glass-Forming Ability of Cu-Zr Binary Alloys. *Acta Physico-chimica Sinica*, **2007**, 23, 895-899		6
150	Band structure of FeBO3: Implications for tailoring the band gap of nanoparticles. *Applied Physics Letters*, **2007**, 91, 253115	3.4	11
149	Fundamental understanding of Na-induced high temperature embrittlement in AlMg alloys. *Philosophical Magazine*, **2007**, 87, 147-157	1.6	14
148	Thermodynamic Investigation of Alkali-Metal-Induced High Temperature Embrittlement in Al-Li Alloys. *Advanced Engineering Materials*, **2007**, 9, 981-986	3.5	

147	Defect structures and ternary lattice site preference of the B2 phase in the Al□NiRu system. *Acta Materialia*, **2007**, 55, 4781-4787	8.4	14
146	First-principles calculations of □-Mg5Si6/□Al interfaces. *Acta Materialia*, **2007**, 55, 5934-5947	8.4	66
145	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
144	MgB2 thin films by hybrid physical□hemical vapor deposition. *Physica C: Superconductivity and Its Applications*, **2007**, 456, 22-37	1.3	98
143	Modified Phase Diagram for the Barium Oxide□Titanium Dioxide System for the Ferroelectric Barium Titanate. *Journal of the American Ceramic Society*, **2007**, 90, 2589-2594	3.8	87
142	Phase stability of hafnium oxide and zirconium oxide on silicon substrate. *Scripta Materialia*, **2007**, 57, 201-204	5.6	15
141	USAMP Magnesium Powertrain Cast Components: Fundamental research summary. *Jom*, **2007**, 59, 43-48	2.1	12
140	Lattice Parameters and Local Lattice Distortions in fcc-Ni Solutions. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2007**, 38, 562-569	2.3	38
139	Modeling of Thermodynamic Properties and Phase Equilibria for the Cu-Mg Binary System. *Journal of Phase Equilibria and Diffusion*, **2007**, 28, 158-166	1	15
138	Defect analysis and thermodynamic modeling of LaCoO3□ *Solid State Ionics*, **2007**, 178, 1027-1032	3.3	26
137	I□V characteristics of the vortex state in MgB2 thin films. *Physical Review B*, **2007**, 76,	3.3	19
136	Thermodynamics of the B□Ca, B□Sr, and B□Ba systems: Applications for the fabrications of CaB6, SrB6, and BaB6 thin films. *Applied Physics Letters*, **2007**, 90, 091914	3.4	7
135	Effects of carbon in MgB2 thin films: Intrinsic or extrinsic. *Applied Physics Letters*, **2007**, 90, 151920	3.4	18
134	Phase stability in □and □rhombohedral boron. *Physical Review B*, **2007**, 75,	3.3	55
133	Lattice dynamics and anomalous bonding in rhombohedral As: First-principles supercell method. *Physical Review B*, **2007**, 76,	3.3	28
132	Effect of substrate-induced strains on the spontaneous polarization of epitaxial BiFeO3 thin films. *Journal of Applied Physics*, **2007**, 101, 114105	2.5	105
131	Applications of computational thermodynamics □the extension from phase equilibrium to phase transformations and other properties. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2007**, 31, 53-74	1.9	43
130	Thermodynamic description and growth kinetics of stoichiometric precipitates in the phase-field approach. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2007**, 31, 303-312	1.9	51

129	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
128	Modeling of Ni□Cr□Mo based alloys: Part II □Kinetics. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2007**, 31, 237-248	1.9	27
127	Thermodynamic modeling of the Ba□Ni□Ti system. *Journal of Alloys and Compounds*, **2007**, 430, 188-193	5.7	7
126	Thermostatics and kinetics of transformations in Pu-based alloys. *Journal of Alloys and Compounds*, **2007**, 444-445, 28-35	5.7	30
125	First-principles elastic constants of □and □Al2O3. *Applied Physics Letters*, **2007**, 90, 101909	3.4	183
124	First-principles study of ternary fcc solution phases from special quasirandom structures. *Physical Review B*, **2007**, 76,	3.3	57
123	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
122	The structural evolution of boron carbide via ab initio calculations. *Applied Physics Letters*, **2007**, 91, 231915	3.4	56
121	Linking length scales via materials informatics. *Jom*, **2006**, 58, 42-50	2.1	31
120	Al2(Mg,Ca) phases in Mg□Al□Ca ternary system: First-principles prediction and experimental identification. *Scripta Materialia*, **2006**, 55, 573-576	5.6	45
119	First-principles calculations on MgO: Phonon theory versus mean-field potential approach. *Journal of Applied Physics*, **2006**, 100, 023533	2.5	22
118	Thermodynamic properties of binary hcp solution phases from special quasirandom structures. *Physical Review B*, **2006**, 74,	3.3	106
117	Intermetallics in the Mg□Ca□Sn ternary system: Structural, vibrational, and thermodynamic properties from first principles. *Physical Review B*, **2006**, 74,	3.3	42
116	A new algorithm for the automation of phase diagram calculation. *Computational Materials Science*, **2006**, 35, 61-74	3.2	17
115	Modeling of Ni□Cr□Mo based alloys: Part I□Phase stability. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2006**, 30, 70-87	1.9	96
114	Thermodynamic modelling of the Zn□Zr system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2006**, 30, 1-13	1.9	53
113	Thermodynamic modeling of the Hf□Si□O system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2006**, 30, 375-386	1.9	68
112	CALPHAD/first-principles re-modeling of the Co□Y binary system. *Journal of Alloys and Compounds*, **2006**, 407, 193-200	5.7	9

111	Thermodynamics modeling of the MgSr and CaMgSr systems. *Journal of Alloys and Compounds*, **2006**, 421, 172-178	5.7	36
110	Thermodynamic modeling of the AlMgNa system. *Journal of Alloys and Compounds*, **2006**, 419, 91-97	5.7	11
109	Contribution of first-principles energetics to the CaMg thermodynamic modeling. *Journal of Alloys and Compounds*, **2006**, 420, 98-106	5.7	31
108	First-principles study of constitutional and thermal point defects in B2 PdIn. *Intermetallics*, **2006**, 14, 248-254	3.5	9
107	First-principles calculations of the ZnZr system. *Acta Materialia*, **2006**, 54, 473-482	8.4	60
106	Finite-temperature thermodynamic and vibrational properties of AlNi compounds via first-principles calculations. *Acta Materialia*, **2006**, 54, 2291-2304	8.4	32
105	Effect of local oxygen activity on NiBaTiO3 interfacial reactions. *Acta Materialia*, **2006**, 54, 3513-3523	8.4	57
104	Thermodynamic modeling of the CaSn system based on finite temperature quantities from first-principles and experiment. *Acta Materialia*, **2006**, 54, 4939-4951	8.4	29
103	First-principles calculations and phenomenological modeling of lattice misfit in Ni-base superalloys. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **2006**, 431, 196-200	5.3	22
102	Phase diagram and thermodynamics of the La2O3Ga2O3 system revisited. *Journal of Physics and Chemistry of Solids*, **2006**, 67, 1901-1907	3.9	22
101	Spectral implementation of an adaptive moving mesh method for phase-field equations. *Journal of Computational Physics*, **2006**, 220, 498-510	4.1	65
100	A combined first-principles calculation and thermodynamic modeling of the FeNa system. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **2006**, 418, 161-171	5.3	12
99	Effect of preheating temperature on the deposition rate of TiCN. *Surface and Coatings Technology*, **2006**, 201, 2818-2821	4.4	5
98	Computational investigations of the bonding layer in CVD-coated WC+Co cutting tools. *Journal of Phase Equilibria and Diffusion*, **2006**, 27, 30-33	1	5
97	Mean-field potential calculations of shock-compressed porous carbon. *Physical Review B*, **2005**, 71,	3.3	8
96	Modification of the thermodynamic model for the MgZr system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2005**, 29, 230-238	1.9	30
95	Contribution of first-principles energetics to AlMg thermodynamic modeling. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2005**, 29, 303-311	1.9	93
94	First-principles calculations and thermodynamic modeling of the NiMo system. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2005**, 397, 288-296	5.3	56

93	Investigations of the bonding layer in commercial CVD coated cemented carbide inserts. *Surface and Coatings Technology*, **2005**, 198, 161-164	4.4	12
92	Ab initio thermodynamic properties of stoichiometric phases in the NiAl system. *Acta Materialia*, **2005**, 53, 1809-1819	8.4	85
91	First-principles study of constitutional point defects in B2 NiAl using special quasirandom structures. *Acta Materialia*, **2005**, 53, 2643-2652	8.4	40
90	First-principles growth kinetics and morphological evolution of Cu nanoscale particles in Al. *Acta Materialia*, **2005**, 53, 2759-2764	8.4	51
89	Thermodynamic Modeling of the Binary BariumOxygen System. *Journal of the American Ceramic Society*, **2005**, 88, 1943-1948	3.8	4
88	Structural stability of NiMo compounds from first-principles calculations. *Scripta Materialia*, **2005**, 52, 17-20	5.6	41
87	Linking first-principles energetics to CALPHAD: An application to thermodynamic modeling of the Al-Ca binary system. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2005**, 36, 5-13	2.3	37
86	Thermoelectric properties of epitaxial and topotaxial NaxCoO2 thin films. *Materials Research Society Symposia Proceedings*, **2005**, 886, 1		1
85	First-Principles Investigation of Laves Phases in Mg-Al-Ca System. *Materials Science Forum*, **2005**, 488-489, 169-176	0.4	11
84	Application of ab initio and CALPHAD thermodynamics to Mo-Ta-W alloys. *Physical Review B*, **2005**, 71,	3.3	53
83	Structural and transport properties of epitaxial NaxCoO2 thin films. *Applied Physics Letters*, **2005**, 87, 172104	3.4	19
82	Phase-field modeling of stress-induced surface instabilities in heteroepitaxial thin films. *Journal of Applied Physics*, **2005**, 98, 044910	2.5	27
81	Progress in the deposition of MgB2thin films. *Superconductor Science and Technology*, **2004**, 17, S196-S201	3.1	30
80	B2 Phases and their Defect Structures: Part I. Ab Initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System. *Materials Research Society Symposia Proceedings*, **2004**, 842, 239		
79	Thermodynamic modeling of the NiAlCaN system. *Journal of Materials Research*, **2004**, 19, 1742-1751	2.5	5
78	Thermodynamic Modeling of the YO1.5ZrO2 System. *Journal of the American Ceramic Society*, **2004**, 87, 1559-1566	3.8	18
77	Thermodynamic calculations of carbonitrides in microalloyed steels. *Scripta Materialia*, **2004**, 50, 601-606	5.6	28
76	An integrated framework for multi-scale materials simulation and design. *Journal of Computer-Aided Materials Design*, **2004**, 11, 183-199		38

75	Modeling of lattice parameter in the Ni-Al system. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2004**, 35, 2313-2321	2.3	28
74	Quantitative interface models for simulating microstructure evolution. *Acta Materialia*, **2004**, 52, 833-848	8.4	41
73	Thermodynamic properties of Al, Ni, NiAl, and Ni3Al from first-principles calculations. *Acta Materialia*, **2004**, 52, 2665-2671	8.4	360
72	A combined CALPHAD/first-principles remodeling of the thermodynamics of Al-Sr: unsuspected ground state energies by rounding up the (un)usual suspects. *Acta Materialia*, **2004**, 52, 2739-2754	8.4	63
71	Three-dimensional phase-field simulations of coarsening kinetics of γ′ particles in binary Ni-Al alloys. *Acta Materialia*, **2004**, 52, 2837-2845	8.4	172
70	First-principles study of binary bcc alloys using special quasirandom structures. *Physical Review B*, **2004**, 69,	3.3	228
69	Ab initio lattice stability in comparison with CALPHAD lattice stability. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2004**, 28, 79-90	1.9	303
68	A computational thermodynamic model of the Ca-Mg-Zn system. *Journal of Alloys and Compounds*, **2004**, 370, 114-122	5.7	31
67	Computational Tools for Designing Ni-Base Superalloys **2004**,		7
66	In situ growth of MgB/sub 2/ thin films by hybrid physical-chemical vapor deposition. *IEEE Transactions on Applied Superconductivity*, **2003**, 13, 3233-3237	1.8	23
65	Deposition and Properties of Superconducting MgB2 Thin Films. *Journal of Superconductivity and Novel Magnetism*, **2003**, 16, 801-806		8
64	Thermodynamic modeling of the Ca-Sr-Zn ternary system. *Journal of Phase Equilibria and Diffusion*, **2003**, 24, 340-346		17
63	JOM-e: The symposium on computational methods in materials education. *Jom*, **2003**, 55, 13-13	2.1	1
62	Creep resistant Mg-Al-Ca alloys: Computational thermodynamics and experimental investigation. *Jom*, **2003**, 55, 40-44	2.1	79
61	Phase relations in the BaO?TiO2 system under highly reducing conditions. *Materials Research Bulletin*, **2003**, 38, 545-553	5.1	9
60	Thermodynamic reactivity of the magnesium vapor with substrate materials during MgB2 deposition. *Physica C: Superconductivity and Its Applications*, **2003**, 397, 87-94	1.3	14
59	Computational investigation of constitutional liquation in Al-Cu alloys. *Acta Materialia*, **2003**, 51, 4447-4459	8.4	17
58	Structure-property relationship of a spray formed Al-Ni-Co alloy. *Acta Materialia*, **2003**, 51, 5199-5209	8.4	13

57	Thermodynamic modeling of the Ca□□Na system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2003**, 27, 235-241	1.9	10
56	Thermodynamic Modeling of Organic Carbonates for Lithium Batteries. *Journal of the Electrochemical Society*, **2003**, 150, A359	3.9	15
55	Phase Field Modeling of Surface Instabilities Induced by Stresses. *Materials Research Society Symposia Proceedings*, **2003**, 795, 247		
54	Effect of external mechanical constraints on the phase diagram of epitaxial PbZr1□TixO3 thin films□hermodynamic calculations and phase-field simulations. *Applied Physics Letters*, **2003**, 83, 1608-1610	3.4	68
53	Superconducting MgB2 thin films on silicon carbide substrates by hybrid physical□hemical vapor deposition. *Applied Physics Letters*, **2003**, 82, 2097-2099	3.4	124
52	Synthesis and thermal stability of a new barium polytitanate compound, Ba1.054Ti0.946O2.946. *Materials Research Bulletin*, **2002**, 37, 467-473	5.1	9
51	An oxygen nonstoichiometry study of barium polytitanates with hollandite structure. *Materials Research Bulletin*, **2002**, 37, 2373-2382	5.1	12
50	Linking phase-field model to CALPHAD: application to precipitate shape evolution in Ni-base alloys. *Scripta Materialia*, **2002**, 46, 401-406	5.6	129
49	Thermodynamic modeling of the indium-palladium system. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2002**, 33, 3597-3603	2.3	10
48	Evaluation of the thermodynamic properties and phase equilibria of the Re-Ta-W system. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2002**, 33, 2781-2787	2.3	3
47	In situ epitaxial MgB2 thin films for superconducting electronics. *Nature Materials*, **2002**, 1, 35-8	27	355
46	Effect of substrate constraint on the stability and evolution of ferroelectric domain structures in thin films. *Acta Materialia*, **2002**, 50, 395-411	8.4	392
45	Effect of electrical boundary conditions on ferroelectric domain structures in thin films. *Applied Physics Letters*, **2002**, 81, 427-429	3.4	195
44	Thermodynamics and thin film deposition of MgB2superconductors. *Superconductor Science and Technology*, **2002**, 15, 451-457	3.1	21
43	Stability and Aging of Candidate Alloys for the Yucca Mountain Project: CALPHAD Results. *Materials Research Society Symposia Proceedings*, **2002**, 757, II4.3.1		
42	Thermodynamic assessment of the Al□a binary system using random solution and associate models. *Journal of Alloys and Compounds*, **2002**, 340, 199-206	5.7	32
41	Modeling Solid-State Phase Transformations and Microstructure Evolution. *MRS Bulletin*, **2001**, 26, 197-202	3.2	32
40	Phase-field model of domain structures in ferroelectric thin films. *Applied Physics Letters*, **2001**, 78, 3878-3880	3.4	276

39	Superconducting properties of nanocrystalline MgB2 thin films made by an in situ annealing process. *Applied Physics Letters*, **2001**, 79, 1840-1842	3.4	70
38	Thermodynamics of the MgB system: Implications for the deposition of MgB2 thin films. *Applied Physics Letters*, **2001**, 78, 3678-3680	3.4	197
37	Computational thermodynamic modeling of the Mg-B system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2001**, 25, 299-303	1.9	42
36	A computational thermodynamic assessment of the Ca-Zn system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2001**, 25, 381-390	1.9	13
35	Thermodynamics of the Cr-Ta-W system by combining the Ab Initio and CALPHAD methods. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2001**, 25, 419-433	1.9	50
34	Evaluation of the thermodynamic properties of the ReTa and ReN systems. *Journal of Alloys and Compounds*, **2000**, 299, 153-162	5.7	37
33	Thermodynamic assessment of the Al-Fe-Si system. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **1999**, 30, 1081-1095	2.3	96
32	Thermodynamic assessment of the Co-Ta system. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **1999**, 23, 339-356	1.9	41
31	A mathematical model for the solute drag effect on recrystallization. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **1998**, 29, 1029-1034	2.3	3
30	A mathematical model for the solute drag effect on recrystallization. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **1998**, 29, 1029-1034	2.3	11
29	Modeling the atomic transport kinetics in high-lead solders. *Journal of Electronic Materials*, **1998**, 27, 1362-1366	1.9	14
28	Thermodynamics of interfacial segregation in solute drag. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1998**, 247, 222-228	5.3	13
27	On the applicability of the Ivantsov growth equation. *Journal of Applied Physics*, **1997**, 82, 4838-4841	2.5	5
26	Towards virtual heat treatment of alloys. *Materials Science and Technology*, **1997**, 13, 740-748	1.5	
25	The transformation phenomenon in Fe-Mo-C alloys: A solute drag approach. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **1997**, 28, 1625-1631	2.3	22
24	Theoretic calculation of ferrite growth in supersaturated austenite in Fe?C alloy. *Acta Materialia*, **1996**, 44, 3855-3867	8.4	18
23	Application of the Le Chatelier principle on gas reactions. *Fluid Phase Equilibria*, **1996**, 121, 167-177	2.5	20
22	Effect of niobium on massive transformation in ultra low carbon steels: a solute drag treatment. *Acta Materialia*, **1996**, 44, 4241-4251	8.4	70

21	A Mathematical Model for the Solute Drag Effect on Recrystallization. *Materials Science Forum*, **1996**, 204-206, 337-342	0.4	
20	Thermodynamics of constrained and unconstrained equilibrium systems and their phase rules. *Journal of Phase Equilibria and Diffusion*, **1995**, 16, 30-35		7
19	Thermodynamic assessment of the Co?Fe?Gd systems. *Journal of Alloys and Compounds*, **1995**, 226, 33-45	5.7	35
18	Solidification and microstructure of a high alloy stainless steel. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **1994**, 25, 1550-1553	2.3	1
17	Reactions in Al2O3?Mg metal matrix composites during prolonged heat treatment at 400, 550 and 600□C. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1993**, 169, 149-157	5.3	11
16	Morphological stability of growing particles and maximum growth rate principle. *Journal of Applied Physics*, **1992**, 71, 4809-4813	2.5	7
15	Uniaxial tension and microstructure of a short alumina fibre-reinforced Al?2Mg alloy. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1991**, 135, 125-127	5.3	7
14	An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy. *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*, **1991**, 22, 1745-1752		74
13	Morphology of cementite decomposition in an fe-cr-c alloy. *Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science*, **1991**, 22, 1753-1759		29
12	Two-Phase Coherent Equilibrium in Multicomponent Alloys. *Journal of Phase Equilibria and Diffusion* , **1991**, 12, 266-274		3
11	Fibre-matrix interactions during fabrication of Al2O3?Mg metal matrix composites. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1990**, 129, 135-145	5.3	50
10	On two-phase coherent equilibrium in binary alloys. *Acta Metallurgica Et Materialia*, **1990**, 38, 561-572		36
9	On the transition from local equilibrium to paraequilibrium during the growth of ferrite in Fe-Mn-C austenite. *Acta Metallurgica*, **1989**, 37, 3157-3163		51
8	Towards a Grid enabled system for multicomponent materials design		1
7	Zentropy Theory for Positive and Negative Thermal Expansion. *Journal of Phase Equilibria and Diffusion*,1	1	2
6	Electronic Structures and Materials Properties Calculations of Ni and Ni-Based Superalloys413-446		
5	A Computational Thermodynamic Analysis of Atmospheric Magnesium Production17-20		
4	Computational Thermodynamics and Experimental Investigation of the Mg-Al-Ca-Sr Alloys421-425		

3 Computational Thermodynamics and Experimental Investigation of Mg-AI-Ca Alloys415-419

2 New Phases in Mg-Al-Ca System427-432

1 Electrons to Phases of Magnesium237-281 1