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The compound energy formalism

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663	Thermodynamic modeling of some aluminium-rare earth binary systems: Al-La, Al-Ce and Al-Nd. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2001 , 25, 583-597	1.9	53
662	The compound energy formalism: applications. <i>Journal of Alloys and Compounds</i> , 2001 , 320, 177-188	5.7	23
661	Point defects in B2 compounds. <i>Journal of Alloys and Compounds</i> , 2001 , 329, 208-213	5.7	14
660	Experimental and Thermodynamic Assessment of the Fe-Gd-Zr System. 2002 , 93, 186-198		8
659	Phase Equilibria in the Si-B-C-N System. 2002 , 1-58		33
658	Thermodynamics of FeSm, FeH, and HSm systems and its application to the hydrogen disproportionation-desorption-recombination (HDDR) process for the system Fe ₁₇ Sm ₂ H ₂ . <i>Journal of Alloys and Compounds</i> , 2002 , 339, 118-139	5.7	35
657	Thermodynamic modeling of the NbSi system. <i>Intermetallics</i> , 2002 , 10, 993-999	3.5	59
656	Thermo-Calc & DICTRA, computational tools for materials science. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2002 , 26, 273-312	1.9	2511
655	Thermodynamic modeling of the FeMoZr system. <i>Acta Materialia</i> , 2002 , 50, 3373-3383	8.4	14
654	Thermodynamic modelling and optimization of the AlCeNd system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2003 , 27, 227-233	1.9	16
653	A description of the effect of short range ordering in the compound energy formalism. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2003 , 27, 403-408	1.9	30
652	Phase equilibria in the CoO-Bi ₂ O ₃ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2003 , 27, 127-132	1.9	6
651	The AlR ₂ Mg (R=Gd, Dy, Ho) systems. Part II: Thermodynamic modelling of the binary and ternary systems. <i>Intermetallics</i> , 2003 , 11, 1135-1151	3.5	75
650	Thermodynamic optimization in the Mg ₂ system. <i>Intermetallics</i> , 2003 , 11, 1183-1188	3.5	60
649	Phase stability of Y + Gd Co-Doped Zirconia. 2003 , 94, 163-170		42
648	Atomic, Electronic, and Magnetic Structure of Iron-Based Sigma-Phases. 2004 , 842, 185		6
647	Study of the La ₂ O ₃ -Ga ₂ O ₃ system by experiment and thermodynamic calculations. 2004 , 25, 437-447		1

646	Assessment of the Sr-Mn-O system. 2004 , 25, 311-319		17
645	Thermodynamic assessment of the BiOxBrOxTaO system. 2004 , 406, 189-200		1
644	Assessment of thermodynamic parameters in the system ZrO ₂ -Y ₂ O ₃ -Al ₂ O ₃ . 2004 , 95, 27-39		94
643	Assessment of the LaBrMnO system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2004 , 28, 191-201	1.9	33
642	Phase equilibria in the CoCuDBi system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2004 , 28, 293-298	1.9	5
641	Thermodynamic analysis of the ternary LaNiO system. <i>Journal of Alloys and Compounds</i> , 2004 , 375, 147-161	5.7	99
640	Thermodynamic modeling of oxidation of AlCrNi alloys. <i>Journal of Alloys and Compounds</i> , 2004 , 381, 99-113	5.7	49
639	Thermodynamic assessment of the CoV and CoVCo system. <i>Journal of Alloys and Compounds</i> , 2004 , 385, 114-118	5.7	14
638	Thermodynamic analysis and assessment of the CeNi system. <i>Intermetallics</i> , 2004 , 12, 1367-1372	3.5	26
637	Development of New Equilibrium Calculation Software: CaTCalc. 2004 , 68, 983-987		1
636	Development of New Equilibrium Calculation Software: CaTCalc. 2005 , 46, 1175-1179		7
635	Thermodynamic description of multi-component multi-phase alloys and its application to the solidification process. 2005 , 413-414, 497-503		3
634	A diffuse interface model of interfaces: Grain boundaries in silicon nitride. <i>Acta Materialia</i> , 2005 , 53, 4758-4764		29
633	Phase equilibria and thermodynamic properties of the ZrO ₂ -GdO _{1.5} -YO _{1.5} system. 2005 , 26, 591-604		71
632	Assessment of the La-Mn-O system. 2005 , 26, 131-151		33
631	Thermodynamics and Microstructure of Co-V8C7 Alloy. 2005 , 492-493, 523-530		2
630	Thermodynamic assessment of MgAlMn phase equilibria, focusing on Mg-rich alloys. 2005 , 96, 857-869		32
629	Thermodynamic assessment of the MgO-Al ₂ O ₃ -Bi ₂ O ₃ system. 2005 , 20, 975-986		41

628	Thermodynamic assessment of the ternary Cu-Pb-D system. 2005 , 96, 879-887		7
627	Experimental investigation and thermodynamic assessment of the V-W-C system. <i>Journal of Alloys and Compounds</i> , 2005 , 395, 68-74	5.7	16
626	Thermodynamic modelling of the M ₆ C carbide in cemented carbides and high-speed steel. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2005 , 29, 91-96	1.9	21
625	Phase relations in the HfO ₂ -ZrO ₂ -Al ₂ O ₃ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2005 , 29, 239-246	1.9	16
624	Thermodynamic analysis of the stable and metastable Co-Ti and Co-Ti-Fe phase diagrams. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2006 , 30, 171-178	1.9	80
623	On the phase relations in the ZrO ₂ -Y ₂ O ₃ -Al ₂ O ₃ system. <i>Journal of Alloys and Compounds</i> , 2006 , 420, 237-245	5.7	30
622	Thermodynamic optimization of the Mg-Ti-B and Mg-Ti systems. <i>Journal of Alloys and Compounds</i> , 2006 , 422, 102-108	5.7	20
621	Phase-field simulation of solidification in multicomponent alloys coupled with thermodynamic and diffusion mobility databases. <i>Acta Materialia</i> , 2006 , 54, 2235-2239	8.4	42
620	Phase diagram and thermodynamics of the La ₂ O ₃ -CaO system revisited. 2006 , 67, 1901-1907		22
619	Thermodynamic evaluation and optimization of the (Na ₂ SO ₄ + K ₂ SO ₄ + Na ₂ S ₂ O ₇ + K ₂ S ₂ O ₇) system. <i>Journal of Chemical Thermodynamics</i> , 2006 , 38, 1568-1583	2.9	31
618	Phase diagram of the ZrO ₂ -Y ₂ O ₃ -Al ₂ O ₃ system. <i>Journal of the European Ceramic Society</i> , 2006 , 26, 233-246	6	72
617	Thermodynamic evaluation of the Co-Ti-W-Ni-Zr system for cemented carbides applications. 2006 , 27, 213-219		10
616	Thermodynamic database for the ZrO ₂ -Y ₂ O ₃ -ZrO ₂ -Al ₂ O ₃ /2 system and application to thermal barrier coatings. 2006 , 27, 343-352		2
615	The effects of applied magnetic fields on the β/β' phase boundary in the Fe-Bi system. 2006 , 39, 2890-2896		22
614	Experimental and thermodynamic evaluation of the Co-Ti-C system. <i>International Journal of Materials Research</i> , 2006 , 97, 1243-1250	0.5	17
613	Thermodynamic modelling of the Ce-Ni system. <i>International Journal of Materials Research</i> , 2006 , 97, 737-743	0.5	4
612	Computational Phase Studies of Oxide Ceramics. 2006 , 45, 17-24		
611	Thermodynamic assessment of the systems La ₂ O ₃ -Al ₂ O ₃ and La ₂ O ₃ -ZrO ₂ . <i>International Journal of Materials Research</i> , 2006 , 97, 1495-1501	0.5	18

610	Thermodynamic assessment of the MnCrO system for solid oxide fuel cell (SOFC) materials. 2006 , 97, 569-578		7
609	Phase diagrams and thermodynamics of rare-earth-doped zirconia ceramics. 2007 , 79, 1731-1753		45
608	Experimental study and thermodynamic assessment of the ZrO ₂ DyO _{1.5} system. <i>International Journal of Materials Research</i> , 2007 , 98, 91-98	0.5	4
607	Calorimetric study and thermodynamic assessment of the SrO-La ₂ O ₃ system. <i>International Journal of Materials Research</i> , 2007 , 98, 574-579	0.5	4
606	Applications of computational thermodynamics II: the extension from phase equilibrium to phase transformations and other properties. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2007 , 31, 53-74	1.9	43
605	Thermodynamic reassessment of the Si ₃ N ₄ -AlN-Al ₂ O ₃ -Bi ₂ O ₃ system Modeling of the SiAlON and liquid phases. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2007 , 31, 269-280	1.9	16
604	Thermodynamic description of the TiO system using the associate model for the liquid phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2007 , 31, 330-342	1.9	60
603	Thermodynamic optimization of the Ru-Sc system. <i>Journal of Alloys and Compounds</i> , 2007 , 427, 148-152	5.7	7
602	Experimental study and thermodynamic calculation of Al-Mg-Br phase equilibria. <i>Intermetallics</i> , 2007 , 15, 506-519	3.5	33
601	Thermodynamic modeling of the Nb-B system. <i>Intermetallics</i> , 2007 , 15, 999-1005	3.5	22
600	Thermodynamic aspects of liquid phase sintering of SiC using Al ₂ O ₃ and Y ₂ O ₃ . <i>International Journal of Materials Research</i> , 2007 , 98, 976-986	0.5	16
599	Thermodynamic modelling in the ZrO ₂ -La ₂ O ₃ -Y ₂ O ₃ -Al ₂ O ₃ system. <i>International Journal of Materials Research</i> , 2007 , 98, 838-846	0.5	30
598	Thermodynamic evaluation of the Nb-Dzr system. 2007 , 360, 242-254		41
597	Thermodynamic evaluation and optimization of the (Na ₂ CO ₃ +Na ₂ SO ₄ +Na ₂ S+K ₂ CO ₃ +K ₂ SO ₄ +K ₂ S) system. <i>Journal of Chemical Thermodynamics</i> , 2007 , 39, 942-960	2.9	23
596	Thermodynamic evaluation and optimization of the (NaCl+Na ₂ SO ₄ +Na ₂ CO ₃ +KCl+K ₂ SO ₄ +K ₂ CO ₃) system. <i>Journal of Chemical Thermodynamics</i> , 2007 , 39, 1001-1021	2.9	39
595	Experimental Investigation and Thermodynamic Modeling of the ZrO ₂ -SmO _{1.5} System. 2007 , 90, 2210-2219		16
594	Thermodynamic calculations of phase equilibria in the neodymium-barium-copper-oxygen system: A model of the Nd _{1+x} Ba _{2-1x} Cu ₃ O _{6+z} phase. 2007 , 81, 1192-1197		2
593	Thermodynamic Database Development of the Mg-Ce-Mn-Y System for Mg Alloy Design. 2007 , 38, 1231-1243		22

592	Critical Evaluation and Thermodynamic Optimization of the Binary Systems in the Mg-Ce-Mn-Y System. 2007 , 28, 342-354		44
591	Thermodynamic assessment of the Cu-Ti-Zr system. I. Cu-Ti system. 2008 , 47, 344-360		36
590	Thermodynamic assessment of the Cu-Ti-Zr system. III. Cu-Ti-Zr system. 2008 , 47, 586-606		9
589	Experimental and Thermodynamic Assessment of the Nb-Ni-Y System. 2008 , 29, 141-155		21
588	Phase equilibria in the $\text{TiO}_2\text{-}0.5\text{ZrO}_2$ system. <i>Journal of the European Ceramic Society</i> , 2008 , 28, 2509-2520		53
587	Vacancy thermodynamics for intermediate phases using the compound energy formalism. <i>Acta Materialia</i> , 2008 , 56, 5255-5262	8.4	13
586	Thermodynamic modeling of the CrPt binary system using the cluster/site approximation coupling with first-principles energetics calculation. <i>Acta Materialia</i> , 2008 , 56, 5796-5803	8.4	8
585	Chapter 2 Phase diagrams in alloy systems. 2008 , 13, 7-80		
584	Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials. 2008 , 22, 4115-4124		136
583	Assessment of thermodynamic functions in the $\text{ZrO}_2\text{-}2\text{O}_3\text{-}2\text{Al}_2\text{O}_3$ system. <i>Journal of Alloys and Compounds</i> , 2008 , 453, 271-281	5.7	23
582	Thermodynamic modeling and experimental investigation of the Ni-rich corner of the NiAlF system. <i>Intermetallics</i> , 2008 , 16, 139-147	3.5	10
581	Theoretical study of the MoRu sigma phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 171-176	1.9	17
580	Assessment of thermodynamic functions in the $\text{ZrO}_2\text{-}2\text{O}_3\text{-}2\text{Al}_2\text{O}_3$ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 142-151	1.9	13
579	Experimental study and thermodynamic modelling of the $\text{ZrO}_2\text{-}0.5\text{O}_2$ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 111-120	1.9	17
578	Thermodynamic modelling of multicomponent cubic Nb, Ti and V carbides/carbonitrides. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 326-337	1.9	20
577	Thermodynamics and kinetics of metallic amorphous phases in the framework of the CALPHAD approach. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 295-314	1.9	29
576	Critical evaluation and thermodynamic optimization of the AlCe, AlY, AlSc and MgSc binary systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 413-422	1.9	96
575	Thermodynamic reassessment of the $\text{Y}_2\text{O}_3\text{-}2\text{Al}_2\text{O}_3\text{-}2\text{Bi}_2\text{O}_3$ system and its subsystems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 399-412	1.9	43

574	Thermodynamic modelling of the CrFeNiD system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 577-592	1.9	44
573	First-principles based calculation of binary and multicomponent phase diagrams for titanium carbonitride. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 543-565	1.9	24
572	Thermochemical modeling of refractory corrosion in slagging coal gasifiers. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 466-469	1.9	8
571	Combined ab-initio and experimental assessment of mixed carbides. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2008 , 32, 615-623	1.9	26
570	Diffusion simulations of MC and M7C3 carbide coarsening in bcc and fcc matrix utilising new thermodynamic and kinetic description. 2008 , 24, 695-704		13
569	Effect of Cr and V on phase equilibria in CoWC based hardmetals. <i>International Journal of Materials Research</i> , 2008 , 99, 287-293	0.5	37
568	Alloy Phase Diagrams Study and Its Application for New Alloy Development. 2008 , 72, 545-556		7
567	Prediction, determination and validation of phase diagrams via the global study of energy landscapes. <i>International Journal of Materials Research</i> , 2009 , 100, 135-152	0.5	71
566	Experimental study of phase relations in the ZrO2-La2O3-Ni2O3 system. <i>International Journal of Materials Research</i> , 2009 , 100, 1521-1528	0.5	11
565	Thermodynamic re-assessment of the TiAlNb system. <i>International Journal of Materials Research</i> , 2009 , 100, 218-233	0.5	28
564	Sinterbonding cobalt-cemented tungsten carbide to tungsten heavy alloys. 2009 , 27, 835-841		14
563	An attempt to correct the quasichemical model. <i>Acta Materialia</i> , 2009 , 57, 5237-5244	8.4	6
562	Determination of phases in the system chromium-platinum (CrPt) and thermodynamic calculations. 2009 , 510-511, 322-327		9
561	A materials research paradigm driven by computation. 2009 , 61, 18-20		11
560	Thermodynamic Assessment of the La-Cr-O System. 2009 , 30, 12-27		15
559	Thermodynamics and Constitution of Mg-Al-Ca-Sr-Mn Alloys: Part I. Experimental Investigation and Thermodynamic Modeling of Subsystems Mg-Ca-Sr and Al-Ca-Sr. 2009 , 30, 146-156		10
558	Thermodynamic Assessment of the La-Fe-O System. 2009 , 30, 351-366		20
557	First-Principles Calculations and CALPHAD Modeling of Thermodynamics. 2009 , 30, 517-534		243

556	Thermodynamic evaluation and optimization of the (Ca+C+O+S) system. <i>Journal of Chemical Thermodynamics</i> , 2009 , 41, 1111-1124	2.9	25
555	Parameters in the compound energy formalism for ionic systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 227-232	1.9	26
554	PANDAT software with PanEngine, PanOptimizer and PanPrecipitation for multi-component phase diagram calculation and materials property simulation. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 328-342	1.9	353
553	Thermodynamic modeling and optimization of the FeNiTi system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 109-123	1.9	86
552	Adding C to the thermodynamic description of the CrFeNiD system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 393-397	1.9	10
551	Thermodynamic modeling of the CrTi binary system using the cluster/site approximation (CSA) coupling with first-principles energetic calculation. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 420-424	1.9	5
550	Thermodynamic investigation of the galvanizing systems, I: Refinement of the thermodynamic description for the FeZn system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 433-440	1.9	34
549	Experimental and thermodynamic evaluation of the miscibility gaps in MC carbides for the CrTiVWZr system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2009 , 33, 530-538	1.9	13
548	Critical assessment and thermodynamic modeling of the binary MgZn, CaZn and ternary MgCaZn systems. <i>Intermetallics</i> , 2009 , 17, 847-864	3.5	69
547	Assessment of thermodynamic functions in the ZrO ₂ Bm2O3Al ₂ O ₃ system. <i>Journal of Alloys and Compounds</i> , 2009 , 475, 86-95	5.7	8
546	Thermodynamic assessment of the CoOxCrO _{1.5} system. <i>Journal of Alloys and Compounds</i> , 2009 , 485, 427-434	5.7	9
545	A universal method for calculating isobaric-isothermal sections of ternary system phase diagrams. 2010 , 84, 525-533		11
544	Thermodynamic Assessment of the Fe-Mn-O System. 2010 , 31, 113-134		42
543	Thermodynamic Evaluation of the Si-C-Al-Y-O System for LPS-SiC Application. 2010 , 31, 238-249		25
542	First-principles density functional calculations for Mg alloys: A tool to aid in alloy development. 2010 , 63, 680-685		41
541	Computational modeling of effects of alloying elements on elastic coefficients. 2010 , 63, 686-691		35
540	Modeling the thermochemical behavior of AmO ₂ . 2010 , 402, 25-29		6
539	Effect of Mg, Ca, and Zn on stability of LiBH ₄ through computational thermodynamics. 2010 , 35, 6812-6821		23

538	Interfacial Reaction between Refractory Materials and Metallurgical Slags containing Fluoride. 2010 , 81, 860-868		40
537	Thermodynamic re-modeling of the Co ₂ Si system. <i>International Journal of Materials Research</i> , 2010 , 101, 1339-1346	0.5	12
536	Phase relations in the ZrO ₂ -Nd ₂ O ₃ -Y ₂ O ₃ system: experimental study and CALPHAD assessment. <i>International Journal of Materials Research</i> , 2010 , 101, 1354-1360	0.5	6
535	Thermodynamic assessment of the Mn-Ni system. <i>International Journal of Materials Research</i> , 2010 , 101, 1222-1231	0.5	6
534	Experimental study and thermodynamic assessment of ternary Mg-Zn-Fe phase relations focused on Mg-rich alloys. <i>Intermetallics</i> , 2010 , 18, 399-405	3.5	26
533	First-principles calculation aided thermodynamic modeling of the Mo-Be system. <i>Intermetallics</i> , 2010 , 18, 574-581	3.5	10
532	The Fe-Ni system: Thermodynamic modelling assisted by atomistic calculations. <i>Intermetallics</i> , 2010 , 18, 1148-1162	3.5	105
531	Thermodynamic assessment of the Al-Mo system and of the Ti-Al-Mo System from 0 to 20 at.% Ti. <i>Intermetallics</i> , 2010 , 18, 1185-1196	3.5	38
530	Thermodynamic assessment of the Cr-Mn system. <i>Journal of Alloys and Compounds</i> , 2010 , 507, 84-92	5.7	20
529	On the fabricability of a composite material containing the FCC matrix with embedded ductile B2 intermetallics. <i>Journal of Alloys and Compounds</i> , 2010 , 505, 459-466	5.7	4
528	Modeling short-range ordering in liquids: The Mg-Al-Sn system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 180-188	1.9	44
527	Thermodynamic assessment of the ZrO ₂ -Nb ₂ O ₃ -Al ₂ O ₃ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 206-214	1.9	16
526	Critical evaluations and thermodynamic optimizations of the Mn-S and the Fe-Mn-S systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 232-244	1.9	11
525	Overview of the applications of thermodynamic databases to steelmaking processes. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 332-362	1.9	72
524	Gibbs: Phase equilibria and symbolic computation of thermodynamic properties. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 393-404	1.9	19
523	On choosing a reference surface for a two-sublattice model. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 452-455	1.9	1
522	Thermodynamic evaluation and optimization of Al-Cd, Al-Tb, Al-Dy, Al-Pr and Al-Er systems using a Modified Quasichemical Model for the liquid. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 456-466	1.9	56
521	A heuristic method to uncover a possible unsoundness of a physical-chemical model. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2010 , 34, 467-477	1.9	

520	Phase-field study for the influence of solute interactions on solidification process in multicomponent alloys. 2010 , 47, 832-838		12
519	Modeling and simulation of nuclear fuel materials. 2010 , 3, 1406		72
518	Thermodynamic description of niobium-rich TiAl alloys. <i>International Journal of Materials Research</i> , 2011 , 102, 692-696	0.5	7
517	Structures of Ceramic Materials: Thermodynamics and Constitution. 2011 , 183-229		
516	Thermodynamic evaluation and optimization of AlTiAl, AlTiCe, AlTiPr, AlTiNd and AlTiM systems using the Modified Quasichemical Model for liquids. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2011 , 35, 30-41	1.9	58
515	Experimental investigation and thermodynamic assessment of the CuSnTi ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2011 , 35, 82-94	1.9	58
514	Thermodynamic investigation of the galvanizing systems, II: Thermodynamic evaluation of the NiZn system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2011 , 35, 276-283	1.9	16
513	Thermodynamic assessment of the FeMnTi system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2011 , 35, 479-491	1.9	73
512	Thermodynamic modeling of the Nb-rich corner in the NbSiB system. <i>Intermetallics</i> , 2011 , 19, 26-34	3.5	15
511	Experimental study and thermodynamic re-assessment of the binary FeTiAl system. <i>Intermetallics</i> , 2011 , 19, 1059-1075	3.5	19
510	Thermodynamic assessment of the CrTi and first assessment of the AlCrTi systems. <i>Intermetallics</i> , 2011 , 19, 1222-1235	3.5	23
509	Thermodynamic modeling and experimental investigation of the magnesium-neodymium-zinc alloys. <i>Intermetallics</i> , 2011 , 19, 1720-1726	3.5	23
508	Stability of Fe-C Martensite Effect of Zener-Ordering. 2011 , 235-240		3
507	Understanding the catalytic effects of H ₂ S on CVD-growth of γ -alumina: Thermodynamic gas-phase simulations and density functional theory. 2011 , 206, 1771-1779		13
506	Experimental investigation and thermodynamic calculation of the phase equilibria in the FeNbTi ternary system. 2011 , 130, 806-814		9
505	Thermodynamic Properties of silicate glasses and melts: VIII. System MgO-Al ₂ O ₃ -SiO ₂ . 2011 , 81, 2051-2061		5
504	A thermodynamic study of the PuAmD system. 2011 , 414, 408-421		30
503	Oxidation of ferritic stainless steel interconnects: Thermodynamic and kinetic assessment. 2011 , 196, 1975-1982		19

502	Up-Date of a Thermodynamic Database of the ZrO ₂ -Gd ₂ O ₃ -Y ₂ O ₃ -Al ₂ O ₃ System for TBC Applications. 2011 , 32, 2-16		21
501	Phase Relations in the ZrO ₂ -Nd ₂ O ₃ -Y ₂ O ₃ System: Experimental Study and Advanced Thermodynamic Modeling. 2011 , 32, 284-297		8
500	Thermodynamic Assessment of the Cu-Fe-O System. 2011 , 32, 498-511		25
499	Thermodynamic analysis of as-cast and heat-treated microstructures of Mg _{1-x} Fe _x Ni ₂ alloys. <i>Acta Materialia</i> , 2011 , 59, 613-622	8.4	32
498	Ta ₂ O ₅ -ZrO ₂ -RuO ₂ system: Experimental study and preliminary thermodynamic description. <i>Journal of the European Ceramic Society</i> , 2011 , 31, 249-257	6	35
497	On the solubility of yttrium in RuO ₂ . 2011 , 110, 054317		5
496	The Solute Redistribution during Solidification of Multi-Component Alloys. 2011 , 311-313, 752-757		
495	Thermodynamic modeling of La ₂ O ₃ -BaO-Mn ₂ O ₃ -Cr ₂ O ₃ for solid oxide fuel cell applications. 2012 , 27, 1915-1926		11
494	Phase relations in the ZrO ₂ -Sm ₂ O ₃ -Y ₂ O ₃ -Al ₂ O ₃ system: experimental investigation and thermodynamic modelling. <i>International Journal of Materials Research</i> , 2012 , 103, 1469-1487	0.5	18
493	An improved magnetic model for thermodynamic modeling. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 39, 11-20	1.9	38
492	Ab initio calculations and thermodynamic modeling for the Fe-Mn-Nb system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 38, 43-58	1.9	36
491	Summary report of XL CALPHAD Rio de Janeiro, Brasil, 2011. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 39, 111-169	1.9	2
490	Thermodynamic properties and phase equilibria in the system MgO-Al ₂ O ₃ -SiO ₂ at high temperatures. 2012 , 61, 809-812		1
489	Ab initio comparative study of the Cu ₁₃ and Cu ₁₃ Nb intermetallic phases in Cu ₁₃ Nb alloys. <i>Journal of Alloys and Compounds</i> , 2012 , 542, 280-292	5.7	23
488	Modelling of metal nano-particle condensation and growth in a reactive atmosphere. <i>International Journal of Materials Research</i> , 2012 , 103, 1015-1024	0.5	2
487	Thermodynamic modeling of the Nb-rich corner in the Nb ₃ Si ₃ Nb system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 36, 82-88	1.9	10
486	A convex hull algorithm for a grid minimization of Gibbs energy as initial step in equilibrium calculations in two-phase multicomponent alloys. 2012 , 61, 54-66		10
485	First-principles calculations and thermodynamic re-modeling of the Hf-W system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 38, 92-99	1.9	15

484	Thermodynamic evaluations and optimizations of binary Mg-light Rare Earth (La, Ce, Pr, Nd, Sm) systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2012 , 38, 100-116	1.9	51
483	Modeling Deep Burn TRISO particle nuclear fuel. 2012 , 430, 181-189		14
482	Thermodynamic Calculations for the Dephosphorization of Silicon Using Molten Slag. 2012 , 64, 973-981		16
481	Thermodynamic Assessments of the Al ₂ O ₃ -Al ₄ C ₃ -AlN and Al ₄ C ₃ -AlN-SiC Systems. 2012 , 33, 357-368		11
480	Computational Thermodynamics: Application to Nuclear Materials. 2012 , 455-470		4
479	A new approach to establish both stable and metastable phase equilibria for fcc ordered/disordered phase transition: application to the AlNi and NiBi systems. 2012 , 135, 94-105		19
478	Phase relations in the ZrO ₂ -Nd ₂ O ₃ -Y ₂ O ₃ -Al ₂ O ₃ system: Experimental study and thermodynamic modeling. <i>Journal of the European Ceramic Society</i> , 2012 , 32, 3171-3185	6	8
477	Thermodynamic modeling of the U-Zr system – A revisit. 2013 , 443, 331-341		48
476	Thermodynamic modeling and experimental study of the Fe-Cr-Zr system. 2013 , 441, 190-202		41
475	Phase Stability in the Mo-Ti-Zr-C System via Thermodynamic Modeling and Diffusion Multiple Validation. 2013 , 44, 3999-4010		6
474	Comparison of Interfacial Reactions Between AlSi7Mg and Alumina Filter After Casting and Spark Plasma Sintering**. 2013 , 15, 1206-1215		5
473	Thermochemical modeling of the U _{1-x} Gd _x O _{2-x/2} phase. 2013 , 443, 588-595		12
472	Thermodynamic modelling of Fe-Sm and Fe-Dy systems. 2013 , 52, 321-328		6
471	First-principles aided thermodynamic modeling of the Nb-Be system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 41, 119-127	1.9	15
470	Thermodynamic modeling of the (U,Lu) ₂ O _{3-x} solid solution phase. 2013 , 433, 227-232		20
469	Ab initio study of the cohesive properties, electronic structure and thermodynamic stability of the NiTi and NiSn intermetallics. <i>Journal of Alloys and Compounds</i> , 2013 , 576, 302-316	5.7	19
468	Phase field simulation for non-isothermal solidification of multicomponent alloys coupled with thermodynamics database. 2013 , 23, 2361-2367		5
467	Coupled thermochemical, isotopic evolution and heat transfer simulations in highly irradiated UO ₂ nuclear fuel. 2013 , 441, 240-251		38

466	Heat capacity for the $\text{Eu}_2\text{Zr}_2\text{O}_7$ and phase relations in the $\text{ZrO}_2\text{-Eu}_2\text{O}_3$ system: Experimental studies and calculations. 2013 , 558, 74-82		19
465	Thermodynamic calculation of the Mg-Mn-Zn and Mg-Mn-Ge systems and re-optimization of their constitutive binaries. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 41, 89-107	1.9	13
464	Thermodynamic description of the layered O3 and O2 structural $\text{LiCoO}_2\text{-CoO}_2$ pseudo-binary systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 41, 6-15	1.9	20
463	Experimental Investigation and Thermodynamic Modeling of the $\text{ZrO}_2\text{-MgO}$ System. 2013 , 15, 618-626		14
462	The Al-Fe-Mn system revisited: An updated thermodynamic description using the most recent binaries. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 43, 86-93	1.9	29
461	Liquid phase formation in the system $\text{Al-N-Al}_2\text{O}_3\text{-Y}_2\text{O}_3$. Part I: Experimental investigations. <i>Journal of the European Ceramic Society</i> , 2013 , 33, 2447-2455	6	10
460	Liquid phase formation in the system $\text{Al}_2\text{O}_3\text{-Y}_2\text{O}_3\text{-AlN}$: Part II. Thermodynamic assessment. <i>Journal of the European Ceramic Society</i> , 2013 , 33, 2457-2463	6	11
459	Thermodynamic evaluation and optimization of the $(\text{Na}+\text{X})$ binary systems ($\text{X}=\text{Ag, Ca, In, Sn, Zn}$) using combined Calphad and first-principles methods of calculation. <i>Journal of Chemical Thermodynamics</i> , 2013 , 66, 22-33	2.9	18
458	CALPHAD modeling of metastable phases in the Al-Mg-Bi system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 43, 94-104	1.9	41
457	Thermodynamic modeling of the Co-Fe-D system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2013 , 41, 76-88	1.9	21
456	The thermochemistry library Thermochemica. 2013 , 67, 266-272		30
455	Defect Chemistry and Phase Equilibria of $(\text{La}_{1-x}\text{Ca}_x)\text{FeO}_3$ -Thermodynamic Modeling. 2013 , 160, F1103-F1108		17
454	A Thermodynamic Database for the $\text{Al}_2\text{O}_3\text{-CaF}_2\text{-CaO}$ System. 2013 , 21-28		
453	. 2013 ,		1
452	Essential Magnesium Alloys Binary Phase Diagrams and Their Thermochemical Data. 2014 , 2014, 1-33		59
451	Thermodynamic Optimization of Mn-Si-C System. 2014 , 641-649		
450	Low-Density Steels: Complex Metallurgy for Automotive Applications. 2014 , 66, 1747-1758		60
449	Experimental Determination of Solid-Liquid Equilibria with Reactive Components: Example of the Fe-Ti-B Ternary System. 2014 , 35, 701-710		11

448	Thermodynamic models of low-temperature Mn-Ni-Si precipitation in reactor pressure vessel steels. 2014 , 4, 101-105		27
447	Structures of Ceramic Materials: Thermodynamics and Constitution. 2014 , 183-229		
446	Process-time Optimization of Vacuum Degassing Using a Genetic Alloy Design Approach. 2014 , 7, 7997-8011	4	
445	The development of phase-based property data using the CALPHAD method and infrastructure needs. 2014 , 3, 158-180		26
444	Mass spectrometric study of thermodynamic properties in the Yb ₂ O ₃ -ZrO ₂ system at high temperatures. 2014 , 28, 109-14		19
443	Alloy gene Gibbs energy partition function and equilibrium holographic network phase diagrams of AuCu ₃ -type sublattice system. 2014 , 24, 3585-3610		5
442	Experimental and computed phase diagrams of the FeRe system. 2014 , 26, 485402		3
441	Thermodynamic calculation of the Al-B system at pressures to 8 GPa. <i>Journal of Superhard Materials</i> , 2014 , 36, 437-439	0.9	2
440	Thermodynamic modeling and experimental investigation of the magnesium–incbamarium alloys. <i>Journal of Alloys and Compounds</i> , 2014 , 593, 71-78	5.7	19
439	Thermodynamics of stable and metastable structures in Fe–C system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 46, 148-158	1.9	58
438	Thermodynamic consistent phase field model for sintering process with multiphase powders. 2014 , 24, 783-789		11
437	Phase equilibria and thermodynamics of Mn–C, Mn–Si, Si–C binary systems and Mn–Si–C ternary system by critical evaluation, combined with experiment and thermodynamic modeling. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 46, 92-102	1.9	27
436	Thermodynamic investigation of the (La _{1-x} Gd _x) ₂ Zr ₂ O ₇ pyrochlore phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 45, 27-32	1.9	3
435	Experimental and thermodynamic study of the Mg–Sn–In–Zn quaternary system. <i>Journal of Alloys and Compounds</i> , 2014 , 588, 75-95	5.7	16
434	Laves phases in the V–Zr system below room temperature: Stability analysis using ab initio results and phase diagram. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 44, 62-69 ¹⁻⁹		6
433	Critical evaluation and thermodynamic optimization of Fe–Cu, Cu–C, Fe–C binary systems and Fe–Cu–C ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 45, 127-137	1.9	38
432	Summary report of CALPHAD XLII San Sebastian, Spain, 2013. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 45, 62-117	1.9	2
431	Experimental investigation and thermodynamic modeling of the ZrO ₂ –MgO–Al ₂ O ₃ system. <i>Journal of the European Ceramic Society</i> , 2014 , 34, 1397-1408	6	12

430	To melting relations in the $\text{La}_2\text{O}_3\text{-Y}_2\text{O}_3\text{-Al}_2\text{O}_3$ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 44, 133-137	1.9	3
429	Thermodynamic calculation of the B-C system at pressures to 24 GPa. <i>Journal of Superhard Materials</i> , 2014 , 36, 358-360	0.9	1
428	Modeling of Thermal Vacancies in Metals within the Framework of the Compound Energy Formalism. 2014 , 35, 780-787		24
427	Thermodynamic evaluation of the Np-Zr system using CALPHAD and ab initio methods. 2014 , 452, 569-577		9
426	First approach for thermodynamic modelling of the high temperature oxidation behaviour of ternary β -strengthened Co-Al-W superalloys. 2014 , 89, 1-5		23
425	Experimental Investigation and Thermodynamic Modeling of the Ni-Rich Part of the Ni-N Phase Diagram. 2014 , 45, 4863-4874		5
424	Modeling of molar volume of the sigma phase involving transition elements. 2014 , 95, 540-550		9
423	Thermodynamic modeling of the Cr-Ni-Ti system using a four-sublattice model for ordered/disordered bcc phases. 2014 , 578, 35-42		9
422	Critical assessment and thermodynamic modeling of Mg-Ca-Zn system supported by key experiments. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 46, 134-147	1.9	16
421	Thermodynamics. 2014 , 588-641		1
420	Thermodynamic Modeling of the Al-Ti-V Ternary System. 2014 , 45, 4155-4164		8
419	Thermodynamic and Experimental Study of the Mg-Sn-Ag-In Quaternary System. 2014 , 35, 284-313		20
418	Thermodynamic evaluation of the copper-rich part of the Cu-Hf-O-S-P system at low temperatures. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 47, 148-160	1.9	4
417	Thermodynamic optimizations on the binary Li-Bi system and ternary Mg-Bi-Pb system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 47, 100-113	1.9	19
416	A description of the effect of short-range ordering in BCC phases with four sublattices. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 45, 40-48	1.9	6
415	Simulation of precipitate evolution in Fe-5 Co-5 Mo with Si addition based on computational thermodynamics. <i>Journal of Alloys and Compounds</i> , 2014 , 587, 158-170	5.7	3
414	Thermodynamic analysis of the Co-Cr-C system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2014 , 46, 226-236	1.9	10
413	Thermodynamic reassessment of U-Cd-D system. 2014 , 452, 397-406		20

412	Thermodynamics of PdMn phases and extension to the FeMnPd system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 314-333	1.9	5
411	Phase-field simulation of the stability of reaction phases at UO ₂ /Zr interface. 2015 , 466, 551-559		4
410	. 2015 ,		
409	The Application of a Recent Thermodynamic Model for Coke Crystallites: Chemisorption of Methyl Groups, Decomposition of Natural Gas, and the Reduction of Metal Oxides. 2015 , 331-338		
408	First-principles calculations, experimental study, and thermodynamic modeling of the Al-Co-Cr system. 2015 , 10, e0121386		11
407	Thermodynamic analysis of the WCoCr system supported by ab initio calculations and verified with quaternary data. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 50, 59-67	1.9	12
406	Experimental determination of the NiCrRu phase diagram and thermodynamic reassessments of the CrRu and NiCrRu systems. <i>Intermetallics</i> , 2015 , 64, 86-95	3.5	8
405	Thermodynamic description of the TiD system. <i>International Journal of Materials Research</i> , 2015 , 106, 439-453	0.5	10
404	Thermodynamics controls amorphous oxide formation: Exclusive formation of a stoichiometric amorphous (Al _{0.33} Zr _{0.67})O _{1.83} phase upon thermal oxidation of AlZr. <i>Acta Materialia</i> , 2015 , 94, 134-142	8.4	20
403	Thermodynamic description of the Ag(Ca, Li, Zn) and Ca(In, Li) binary systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 50, 68-81	1.9	19
402	Thermodynamic assessment of the VD system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 144-160	1.9	17
401	Critical evaluation and thermodynamic optimization of the VD system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 241-251	1.9	16
400	Thermodynamic assessment of the AlCuZn system, part II: AlCu binary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 252-260	1.9	29
399	Computational Thermodynamics and Kinetics-Based ICME Framework for High-Temperature Shape Memory Alloys. 2015 , 1, 429-449		1
398	The implementation of an algorithm to calculate thermodynamic equilibria for multi-component systems with non-ideal phases in a free software. 2015 , 101, 127-137		37
397	Incorporating the CALPHAD sublattice approach of ordering into the phase-field model with finite interface dissipation. <i>Acta Materialia</i> , 2015 , 88, 156-169	8.4	67
396	C-vacancy concentration in cementite, Fe ₃ C1□ in equilibrium with □-Fe[C] and □Fe[C]. <i>Acta Materialia</i> , 2015 , 86, 374-384	8.4	16
395	A new self-consistent model for thermodynamics of binary solutions. 2015 , 108, 27-30		4

394	Assessments of molar volume of the binary C14 Laves phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 50, 82-91	1.9	2
393	Experimental investigation of phase equilibria in the ZrNbCr system at 1573K and 1373K. 2015 , 465, 626-632		2
392	Holographic alloy positioning design system and holographic network phase diagrams of AuCu system. 2015 , 25, 885-906		3
391	Thermal Stability of Intermetallic Phases in Fe-rich Fe-Cr-Ni-Mo Alloys. 2015 , 46, 3900-3908		5
390	Thermodynamic modelling of the general NiAs-type structure: A study of first principle energies of formation for binary Ni-containing B8 compounds. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 50, 174-181	1.9	6
389	Critical Evaluation and Thermodynamic Optimization of the Ti-C-O System and Its Applications to Carbothermic TiO ₂ Reduction Process. 2015 , 46, 1782-1801		27
388	New experimental investigations of phase relations in the Yb ₂ O ₃ /Al ₂ O ₃ and ZrO ₂ /Nb ₂ O ₃ /Al ₂ O ₃ systems and assessment of thermodynamic parameters. <i>Journal of the European Ceramic Society</i> , 2015 , 35, 2855-2871	6	6
387	Thermodynamic calculations of the MnBn, MnBr and MgMn{Sn, Sr} systems. 2015 , 9, 681-692		7
386	On the interpretation of chemical potentials computed from equilibrium thermodynamic codes. 2015 , 464, 48-52		10
385	Thermodynamic modeling of AlO _x (X = Si,Zr). 2015 , 464, 170-184		16
384	Thermodynamic modelling of the NbNiBi phase diagram based on the 1073 K isothermal section using ab initio calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 57-66	1.9	6
383	Quantitative Defect Chemistry Analysis and Electronic Conductivity Prediction of La _{0.8} Sr _{0.2} MnO ₃ Perovskite. 2015 , 162, E134-E140		14
382	Experimental investigation and thermodynamic modeling of the ZrO ₂ /MnO system. <i>Journal of the European Ceramic Society</i> , 2015 , 35, 3623-3632	6	6
381	Development of thermodynamic database for high Mn/high Al steels: Phase equilibria in the FeMnAl system by experiment and thermodynamic modeling. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 89-103	1.9	27
380	Thermodynamic modeling of the LaMgZn, PrMgZn and SmMgZn system. <i>Journal of Alloys and Compounds</i> , 2015 , 652, 415-425	5.7	9
379	Thermodynamic Modeling of the Fe-Mn-C and the Fe-Mn-Al Systems Using the Modified Quasichemical Model for Liquid Phase. 2015 , 36, 453-470		18
378	Thermodynamic modeling of the YMgZn, GdMgZn, TbMgZn, DyMgZn, HoMgZn, ErMgZn, TmMgZn and LuMg-Zn systems. <i>Journal of Alloys and Compounds</i> , 2015 , 652, 426-443	5.7	19
377	Thermodynamic assessment of the AlCuZn system, part I: CuZn binary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 51, 224-232	1.9	17

376	Strong coupling effects during Cu/In/Ni interfacial reactions at 280°C. <i>Intermetallics</i> , 2015 , 58, 91-97	3.5	8
375	Thermodynamic evaluation and optimization of the (NaNO ₃ +KNO ₃ +Na ₂ SO ₄ +K ₂ SO ₄) system. <i>Journal of Chemical Thermodynamics</i> , 2015 , 83, 12-26	2.9	14
374	Thermodynamic assessment of the MnS and FeMnS systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 48, 95-105	1.9	16
373	Experimental investigation and thermodynamic assessment of the MgCdAg system focused on Mg-rich region. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015 , 48, 43-54	1.9	7
372	A thermodynamic approach for identifying the conditions for gasless detonation. 2015 , 149-150, 27-33		
371	Thermodynamic assessment of the ULaD system. 2015 , 456, 142-150		10
370	Thermodynamic reassessment of Nb-Ni-Ti system with order-disorder model. <i>Journal of Alloys and Compounds</i> , 2015 , 619, 733-747	5.7	17
369	Ab initio study of the compound-energy modeling of multisublattice structures: The (hP6) Ni ₂ In-type intermetallics of the NiThSn system. <i>Journal of Alloys and Compounds</i> , 2015 , 619, 464-473	5.7	4
368	Atomistically Informed Extended Gibbs Energy Description for Phase-Field Simulation of Tempering of Martensitic Steel. 2016 , 9,		5
367	A Combined Experimental and Computational Thermodynamic Investigation of the UThD System. 2016 , 99, 2197-2209		6
366	Thermodynamics of the Fe-N and Fe-N-C Systems: The Fe-N and Fe-N-C Phase Diagrams Revisited. 2016 , 47, 6173-6186		28
365	References. 244-247		
364	Thermodynamic calculation of the phase diagram for the AlBC system at pressure 7.7 GPa. <i>Journal of Superhard Materials</i> , 2016 , 38, 423-426	0.9	2
363	Measurement of the oxygen partial pressure and thermodynamic modeling of the UNdD system. 2016 , 473, 272-282		7
362	Thermodynamic description of the FeMnCaMgS system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 53, 55-61	1.9	4
361	Application of thermochemical modeling to assessment/evaluation of nuclear fuel behavior. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 55, 47-51	1.9	9
360	Thermodynamic description of the Cr-Mn-Si system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 55, 181-188	1.9	3
359	Critical evaluation and thermodynamic optimization of the U-Pb and U-Sb binary systems. 2016 , 480, 216-222		2

358	Precipitation in Microalloyed Steel by Model Alloy Experiments and Thermodynamic Calculations. 2016 , 47, 4806-4817		9
357	Phase diagram of the BB ₂ O ₃ system at pressures to 24 GPa. <i>Journal of Superhard Materials</i> , 2016 , 38, 216-218	0.9	5
356	Thermodynamic modeling of the Al-Cr-Ni system over the entire composition and temperature range. <i>Journal of Alloys and Compounds</i> , 2016 , 688, 422-435	5.7	55
355	Experimental Investigation and CALPHAD Assessment of the Eutectic Trough in the System NiAl-Cr-Mo. 2016 , 37, 592-600		13
354	The OpenCalphad thermodynamic software interface. 2016 , 125, 188-196		30
353	Thermodynamic prediction of the effect of CO ₂ to the stability of (La _{0.8} Sr _{0.2}) _{0.98} MnO _{3-δ} system. 2016 , 41, 10239-10248		27
352	Ab initio energetics for modeling phase stability of the Np-U system. 2016 , 479, 260-270		2
351	Experimental investigation and thermodynamic re-assessment of the AlMoNi system. <i>Journal of Alloys and Compounds</i> , 2016 , 674, 305-314	5.7	16
350	High-temperature phase transformations in strongly metastable austenitic-martensitic CrMnNi-N-C cast steels. <i>Journal of Alloys and Compounds</i> , 2016 , 686, 511-521	5.7	6
349	Statistical physics of multicomponent alloys using KKR-CPA. 2016 , 93,		20
348	Experimental investigation and thermodynamic evaluation of the CdZr ternary system. 2016 , 6, 100122-100135		3
347	Thermodynamic stability maps for the La _{0.6} Sr _{0.4} Co _{0.2} Fe _{0.8} O _{3-δ} system for application in solid oxide fuel cells. 2016 , 336, 351-359		22
346	The (α + ε) Two-Phase Equilibrium in the Fe-N-C System: Experimental Investigations and Thermodynamic Calculations. 2016 , 47, 4411-4424		7
345	Thermodynamic investigation on phase formation in the AlSi rich region of AlSi system. 2016 , 102, 78-90		41
344	Thermodynamic modeling of the SrCoFe system. 2016 , 292, 88-97		6
343	Experimental investigation of phase relations and thermodynamic properties in the system ZrO ₂ -Eu ₂ O ₃ -Al ₂ O ₃ . <i>Journal of the European Ceramic Society</i> , 2016 , 36, 1455-1468	6	3
342	Thermodynamically consistent microstructure prediction of additively manufactured materials. 2016 , 57, 359-370		40
341	A thermodynamic model for non-stoichiometric cementite; the Fe- ϵ phase diagram. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 52, 38-46	1.9	12

340	Thermodynamic modelling and in-situ neutron diffraction investigation of the (Nd + Mg + Zn) system. <i>Journal of Chemical Thermodynamics</i> , 2016 , 94, 43-51	2.9	5
339	Cohesive properties of (Cu,Ni)(In,Sn) intermetallics: Database, electron-density correlations and interpretation of bonding trends. 2016 , 93, 40-51		5
338	Thermodynamic description of the AgCl-CuCl ₂ -InCl ₃ -NaCl system. <i>Journal of Alloys and Compounds</i> , 2016 , 663, 885-898	5.7	8
337	Thermodynamic Assessment of the Fe-Ca-S, Fe-Mg-O and Fe-Mg-S Systems. 2016 , 37, 277-292		7
336	Methods for storage of Gibbs energy data of substances. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 53, 146-150	1.9	3
335	Thermodynamic evaluation and optimization of the (KF+YF ₃), (KCl+YCl ₃) and (YF ₃ +YbF ₃) binary systems. <i>Journal of Chemical Thermodynamics</i> , 2016 , 98, 242-253	2.9	6
334	Critical Evaluation and Thermodynamic Optimization of the Na ₂ O-FeO-Fe ₂ O ₃ -SiO ₂ System. 2016 , 47, 291-308		7
333	Thermodynamic re-assessment of the Co-Ti system supported by first-principles calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2016 , 52, 1-7	1.9	24
332	Thermodynamic modelling and in-situ neutron diffraction investigation of the (Ce + Mg + Zn) system. <i>Journal of Chemical Thermodynamics</i> , 2016 , 93, 242-254	2.9	6
331	Critical evaluation and thermodynamic optimization of the (U + Bi), (U + Si) and (U + Sn) binary systems. <i>Journal of Chemical Thermodynamics</i> , 2016 , 92, 158-167	2.9	14
330	Application of Thermodynamic Calculations to the Pyro-refining Process for Production of High Purity Bismuth. 2017 , 48, 73-90		4
329	Oxidation of iron at 600 °C [Experiments and simulations. 2017 , 68, 133-142		17
328	Thermodynamics of the Mg-Mn-O system [Modeling and heat capacity measurements. 2017 , 100, 1661-1672		12
327	Combining thermodynamic modeling and 3D printing of elemental powder blends for high-throughput investigation of high-entropy alloys [Towards rapid alloy screening and design. 2017 , 688, 180-189		100
326	An improved sampling strategy for global energy minimization of multi-component systems. 2017 , 130, 282-291		9
325	Phase equilibria in the Nb-Ti side of the Nb ₅ Ti ₃ system at 1200 °C and its oxidation behavior. <i>Journal of Alloys and Compounds</i> , 2017 , 704, 311-321	5.7	18
324	Compositional screening of Zr-Nb-Mo alloys with CALPHAD-type model for promising bio-medical implants. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 56, 196-206	1.9	3
323	Thermodynamic description of the Fe-Ca-O-S system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 57, 118-125	1.9	4

322	Experimental investigation and thermodynamic evaluation of the CeHfD ternary system. 2017 , 100, 3757-3770		8
321	Quantitative evaluation of site preference in Dy-substituted Nd ₂ Fe ₁₄ B. <i>Journal of Alloys and Compounds</i> , 2017 , 721, 476-481	5-7	9
320	PrecHiMn-4A thermodynamic database for high-Mn steels. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 56, 49-57	1.9	24
319	Software tools for high-throughput CALPHAD from first-principles data. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 58, 70-81	1.9	37
318	An assessment of the Ti-V-O system. <i>Journal of Alloys and Compounds</i> , 2017 , 722, 365-374	5-7	9
317	Experimental and thermodynamic study of the Mg-Sn-Ca-Sr quaternary system: Part I-Mg-Sn-Ca ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 58, 6-16	1.9	10
316	High-temperature thermochemical energy storage based on redox reactions using Co-Fe and Mn-Fe mixed metal oxides. 2017 , 253, 6-14		41
315	Formation of Corundum, Magnesium Titanate, and Titanium(III) Oxide at the Interface between Rutile and Molten Al or AlSi7Mg0.6 Alloy . 2017 , 19, 1700106		3
314	Thermodynamic assessments of the Cr-Si and Al-Cr-Si systems. <i>Journal of Alloys and Compounds</i> , 2017 , 708, 887-902	5-7	16
313	High-Throughput Thermodynamic Modeling and Uncertainty Quantification for ICME. 2017 , 69, 886-892		24
312	Multiphase Characterization of Cu-In-Sn Alloys with 17 at.% Cu and Comparison with Calculated Phase Equilibria. 2017 , 38, 276-287		1
311	Phase diagrams for understanding gold-seeded growth of GaAs and InAs nanowires. 2017 , 50, 134002		14
310	First-principles calculations and thermodynamic modeling of the Sn-Ta system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 57, 46-54	1.9	3
309	Cohesive Properties of Cu-X and Ni-X (In, Sn) Intermetallics: Ab Initio Systematics, Correlations and Universality Features. 2017 , 38, 257-267		2
308	Effect of SO ₂ Poisoning on the Electrochemical Activity of La _{0.6} Sr _{0.4} Co _{0.2} Fe _{0.8} O _{3-λ} Cathodes of Solid Oxide Fuel Cells. 2017 , 164, F514-F524		22
307	Quantification of process variables for carbothermic synthesis of UC _{1-x} N _x fuel microspheres. 2017 , 483, 176-191		16
306	An assessment of the Ca-V-O system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 56, 29-40	1.9	9
305	A comparison of Redlich-Kister polynomial and cubic spline representations of the chemical potential in phase field computations. 2017 , 128, 127-139		12

304	Thermodynamic re-assessment of the Al-Co-W system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 59, 112-130	1.9	28
303	SrZrO ₃ Formation at the Interlayer/Electrolyte Interface during (La _{1-x} Sr _x) _{1-y} FeyO ₃ Cathode Sintering. 2017 , 164, F3097-F3103		32
302	New Thermodynamic Assessment of the Fe-Y System. 2017 , 38, 684-699		15
301	On the stochastic phase stability of TiAlC-CrAlC. 2017 , 7, 5138		13
300	Liquidus Projection and Thermodynamic Modeling of a Sn-Ag-Zn System. 2017 , 46, 6910-6921		0
299	Temperature hysteresis of the order-disorder transition in carbon-supersaturated α -Fe. 2017 , 96,		17
298	Coexistence of conversion and intercalation mechanisms in lithium ion batteries: Consequences for microstructure and interaction between the active material and electrolyte. <i>International Journal of Materials Research</i> , 2017 , 108, 971-983	0.5	3
297	Thermodynamic modeling of the V-Si-B system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 59, 199-206	1.9	9
296	Coupled Experimental Study and Thermodynamic Optimization of the K ₂ O-MgO and K ₂ O-MgO-SiO ₂ Systems. 2017 , 48, 2788-2803		4
295	Applications of Multicomponent Databases to the Improvement of Steel Processing and Design. 2017 , 38, 916-927		7
294	Thermodynamic Assessments of the Fe-Si-Cr and Fe-Si-Mg Systems. 2017 , 48, 4342-4355		8
293	Thermodynamic Modeling of the Al-Cr-Mn Ternary System. 2017 , 48, 1383-1401		5
292	Thermodynamic description of the ZrO ₂ -TiO ₂ -Al ₂ O ₃ system based on experimental data. <i>Journal of the European Ceramic Society</i> , 2017 , 37, 3461-3469	6	10
291	Critical evaluation and thermodynamic optimization of the Na ₂ O-FeO-Fe ₂ O ₃ -Al ₂ O ₃ -Bi ₂ O ₃ system. <i>Journal of the European Ceramic Society</i> , 2017 , 37, 787-800	6	8
290	Formation of different alumina phases and magnesium aluminate spinel during contact of molten AlSi ₇ Mg _{0.6} alloy with mullite and amorphous silica. 2017 , 114, 79-87		4
289	Phase formations in low density high entropy alloys. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017 , 56, 19-28	1.9	29
288	Binary Phase Diagrams and Thermodynamic Properties of Silicon and Essential Doping Elements (Al, As, B, Bi, Ga, In, N, P, Sb and Tl). 2017 , 10,		35
287	Thermodynamic Modeling of Fe ₂ S Ternary System. 2017 , 57, 782-790		11

286	DGM News. <i>International Journal of Materials Research</i> , 2018 , 109, 182-182	0.5	6
285	The Application of Computational Thermodynamics to the Cathode-Electrolyte in Solid Oxide Fuel Cells. 2018 , 281-335		1
284	Thermodynamic modeling of the K ₂ O-Al ₂ O ₃ and K ₂ O-MgO-Al ₂ O ₃ systems with emphasis on δ and δ' -aluminas. <i>Journal of the European Ceramic Society</i> , 2018 , 38, 3188-3200	6	4
283	Modeling solid-state detonation based on thermochemical equilibrium calculations. 2018 , 1-6		
282	Experimental investigation and thermodynamic modelling of LiF-NdF ₃ -DyF ₃ system. <i>Journal of Alloys and Compounds</i> , 2018 , 753, 388-394	5.7	5
281	Contribution to the thermodynamic description of the corium Γ U-Zr-O system. 2018 , 501, 104-131		26
280	A CALPHAD assessment of the AlMn Γ system supported by ab initio calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 60, 231-239	1.9	8
279	Thermodynamic modeling of the Al-C-Mn system supported by ab initio calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 60, 222-230	1.9	11
278	Thermodynamic investigation of the Al-Fe-Mn system over the whole composition and wide temperature ranges. <i>Journal of Alloys and Compounds</i> , 2018 , 742, 1046-1057	5.7	16
277	Computational phase diagrams for the Nd-based magnets based on the combined ab initio/CALPHAD approach. 2018 , 154, 305-310		9
276	Characterization of a functionally graded material of Ti-6Al-4V to 304L stainless steel with an intermediate V section. <i>Journal of Alloys and Compounds</i> , 2018 , 742, 1031-1036	5.7	48
275	Revised thermodynamic description of the Fe-Cr system based on an improved sublattice model of the ϵ phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 60, 16-28	1.9	33
274	Experimental investigation and thermodynamic assessment of the Al-Co-Ni system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 61, 198-210	1.9	17
273	Phase Diagram of the BBN System at Pressures up to 24 GPa: Experimental Study and Thermodynamic Analysis. 2018 , 122, 8505-8509		10
272	High-Throughput Description of Infinite Composition Structure-Property-Performance Relationships of Lithium-Manganese Oxide Spinel Cathodes. 2018 , 30, 2287-2298		15
271	Thermodynamic Description of the Quaternary Ag-Bi-Cu-Sn System. 2018 , 47, 212-224		1
270	Experimental investigation of phase relations and thermodynamic properties in the ZrO ₂ -TiO ₂ system. 2018 , 101, 386-399		8
269	Solid-liquid equilibria for a pyrrolidinium-based common-cation ternary ionic liquid system, and for a pyridinium-based ternary reciprocal ionic liquid system: an experimental study and a thermodynamic model. 2017 , 20, 637-657		8

268	Design of Materials Processing Using Computational Thermodynamics. 2018 , 27-45		
267	Applications of Thermodynamic Database to the Kinetic Steelmaking Process Simulations. 2018 , 47-66		4
266	Thermodynamic assessment of the pseudoternary Na ₂ O-Al ₂ O ₃ -Bi ₂ O ₃ system. 2018 , 101, 928-948		8
265	Improving Steel and Steelmaking in Ionic Liquid Database for Alloy Process Design. 2018 , 7, 195-201		2
264	Thermodynamic Modeling of the SFCA Phase Ca ₂ (Fe,Ca) ₆ (Fe,Al,Si) ₆ O ₂₀ . 2018 , 58, 259-266		19
263	Ordering of Primary Carbonitrides in an Austenitic Steel Revealed by Transmission Electron Microscopy and Atom Probe Tomography. 2018 , 11,		1
262	Implementation of an Effective Bond Energy Formalism in the Multicomponent Calphad Approach. 2018 , 123, 1-33		4
261	Modelling microstructure evolution during casting, homogenization and ageing heat treatment of Al-Mg-Si-Cu-Fe-Mn alloys. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 63, 164-184	1.9	13
260	Effect of Thermal Vacancy on Thermodynamic Behaviors in BCC W Close to Melting Point: A Thermodynamic Study. 2018 , 11,		5
259	The Ta-B system: Key experiments and thermodynamic modeling. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 63, 107-115	1.9	4
258	Critical Evaluation and Optimization of the Fe-N, Mn-N and Fe-Mn-N Systems. 2018 , 39, 650-677		6
257	A first-principles based description of the Hf-Ni system supported by high-temperature synchrotron experiments. 2018 , 668, 142-151		4
256	Thermodynamic Evaluation of the Co-Al-C System by Coupling Ab Initio Calculations and CALPHAD Approach. 2018 , 39, 538-548		1
255	Thermodynamic reassessment of the Ni ₃ Al system using ab-initio data for end-member compound energies. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 62, 42-48	1.9	3
254	A thermodynamic description for water, hydrogen fluoride and hydrogen dissolutions in cryolite-base molten salts. 2018 , 20, 17324-17341		6
253	Study of the solubility of Pb, Bi and Sn in aluminum by mixed CALPHAD/DFT methods: Applicability to aluminum machining alloys. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2018 , 61, 275-287	1.9	4
252	Thermodynamic modeling of the K-KCl and Mg-MgCl ₂ binary systems using the CALPHAD method. 2018 , 170, 1039-1042		3
251	Ocean of Data: Integrating First-Principles Calculations and CALPHAD Modeling with Machine Learning. 2018 , 39, 635-649		19

250	Thermodynamic Assessments of the Ni-Cr-Ti System and Atomic Mobility of Its fcc Phase. 2018 , 39, 597-609	4
249	Investigation on Phase Stability of $Al_xCo_{0.2}Cr_{0.2}Ni_{0.2}Ti_{0.4}$ High Entropy Alloys. 2018 , 39, 610-622	6
248	Ab-initio based search for late blooming phase compositions in iron alloys. 2018 , 509, 225-236	12
247	Probing long-range ordering in nickel-base alloys with proton irradiation. <i>Acta Materialia</i> , 2018 , 156, 446-462	8.4 19
246	Formation of core (M7C3)-shell (M23C6) structured carbides in white cast irons: A thermo-kinetic analysis. 2018 , 154, 111-121	8
245	Thermodynamic assessment of the Fe-Te system. Part II: Thermodynamic modeling. <i>Journal of Alloys and Compounds</i> , 2018 , 767, 883-893	5-7 9
244	Cu-Be-Co System: Verification of the High-Temperature Phase Equilibria and Thermodynamic Modeling of the Low-Temperature Phase Relations Involving Ordered Phase. 2018 , 56, 546-555	4
243	Thermodynamic Optimization of the Ag-Bi-Cu-Ni Quaternary System: Part I, Binary Subsystems. 2018 , 47, 4056-4069	1
242	Experimental study of phase equilibria in the Al_2O_3 - MgO - TiO_2 system and thermodynamic assessment of the binary MgO - TiO_2 system. 2018 , 101, 5198-5218	9
241	The Role of Research in Pyrometallurgy Technology Development From Fundamentals to Process Improvements Future Opportunities. 2018 , 19-37	2
240	A Review of Calphad Modeling of Ordered Phases. 2018 , 39, 678-693	22
239	Thermodynamic optimization of the K_2O - Al_2O_3 - SiO_2 system. 2018 , 44, 16712-16724	18
238	Size, shape, and compositional effects on the order-disorder phase transitions in Au-Cu and Pt-M (M=Fe, Co, and Ni) nanocluster alloys. 2018 , 29, 345701	7
237	High-Temperature Oxidation Behavior of a Novel Co-Base Superalloy. 2018 , 49, 4058-4069	20
236	Thermodynamic Modelling of Iron Ore Sintering Reactions. 2019 , 9, 361	13
235	Thermodynamic assessment of the solar-to-fuel performance of $La_{0.6}Sr_{0.4}Mn_{1-y}Cr_yO_3$ - perovskite solid solution series. <i>Acta Materialia</i> , 2019 , 178, 163-172	8.4 8
234	Thermodynamic description of the K, Be//F, Cl salt system with first-principles calculations. 2019 , 292, 111384	2
233	Fast prediction of the quasi phase equilibrium in phase field model for multicomponent alloys based on machine learning method. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 66, 101644	1.9 3

232	Thermodynamic assessment of the NiTi system. 2019 , 54, 11304-11319		10
231	Aluminum-doped strontium ferrites for a two-step solar thermochemical air separation cycle: Thermodynamic characterization and cycle analysis. 2019 , 188, 775-786		13
230	ESPEI for efficient thermodynamic database development, modification, and uncertainty quantification: application to CuMg. 2019 , 9, 618-627		22
229	Thermodynamic assessment of the FeNiTi system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 67, 101672	1.9	
228	Solid-Liquid Equilibria for Hexafluorophosphate-Based Ionic Liquid Quaternary Mixtures and Their Corresponding Subsystems. 2019 , 123, 8954-8969		3
227	Thermodynamic assessment of the REZn (RE = Dy, Er, Ho, Tb) binaries as a starting step for a MgZnZrRare earth multicomponent database. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 67, 101676	1.9	0
226	Degradation and reduction of small punch creep life of service-exposed Super304H steel. 2019 , 33, 5243-5250		8
225	Basic Oxygen Furnace: Assessment of Recent Physicochemical Models. 2019 , 50, 2647-2666		7
224	Experimental determination and thermodynamic optimization of the CuClZnCl ₂ , ZnCl ₂ FeCl ₃ , CuClFeCl ₃ , CuClCuCl ₂ , FeCl ₂ FeCl ₃ , FeCl ₂ TuCl ₂ and CuClBbCl ₂ phase equilibria. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 67, 101667	1.9	2
223	Quasi In Situ Growth Observation and Precipitation Kinetics Assessment of the Mn Phase in Fe-30Mn-9Al-1C Steel. 2019 , 71, 4715-4725		1
222	Thermodynamics of solute capture during the oxidation of multicomponent metals. <i>Acta Materialia</i> , 2019 , 181, 584-594	8.4	7
221	On Gibbs Energy for the Metastable bcc_A2 Phase with a Thermal Vacancy in Metals and Alloys. 2019 , 12,		2
220	Modelling of phase equilibria of LiFePO ₄ -FePO ₄ olivine join for cathode material. 2019 , 97, 2224-2233		5
219	Identifying rhenium substitute candidate multiprincipal-element alloys from electronic structure and thermodynamic criteria. 2019 , 34, 3296-3304		7
218	Thermodynamic assessment and experimental investigation of the systems AlBeMn and AlBeMnNi. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 66, 101621	1.9	11
217	Phase relations in the ZrO ₂ -La ₂ O ₃ -Nd ₂ O ₃ system: Experimental studies and phase modeling. 2019 , 102, 7628-7644		5
216	Heat capacity measurement of Zr ₂ Fe and thermodynamic re-assessment of the FeZr system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 66, 101625	1.9	14
215	An updated thermodynamic description of the W-Co and W-Co-Cr systems with focus on ground state intermetallic phases. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 66, 101626	1.9	2

214	Numerical Simulation of the SrZrO ₃ Formation in Solid Oxide Fuel Cells. 2019 , 48, 5510-5515		1
213	Quantified uncertainty in thermodynamic modeling for materials design. <i>Acta Materialia</i> , 2019 , 174, 9-15	3.4	21
212	Combined Cr and S poisoning of La _{0.8} Sr _{0.2} MnO ₃ - λ (LSM) cathode of solid oxide fuel cells. 2019 , 312, 202-212		16
211	Critical evaluation and thermodynamic modeling of the Al-Co-Fe system. <i>Journal of Alloys and Compounds</i> , 2019 , 794, 553-568	5-7	8
210	Thermodynamic analysis of the Co-W system. 2019 , 54, 10261-10269		4
209	Thermodynamic Modeling of the La-Co-O System. 2019 , 40, 219-234		2
208	Phase equilibria and thermodynamic evaluation of the Fe-Ti-V-O system in air. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 65, 141-154	1.9	1
207	Influence of synthesis method on microstructure and mechanical behavior of Co-free AlCrFeNi medium-entropy alloy. <i>Intermetallics</i> , 2019 , 108, 45-54	3-5	23
206	Integrated modeling of molar volume of the sigma phase aided by first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2019 , 791, 994-1004	5-7	4
205	Thermodynamic assessment of the hollandite high-level radioactive waste form. 2019 , 102, 6284-6297		5
204	Thermodynamic assessment of the Al ₂ O ₃ -MgO-TiO ₂ system. <i>Journal of Alloys and Compounds</i> , 2019 , 790, 1137-1148	5-7	8
203	Thermodynamic modelling of the Ni-V system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 65, 273-281	1.9	2
202	Thermodynamic modeling of the chromium-yttrium-oxygen system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 64, 1-10	1.9	1
201	Thermodynamic Modeling of the SFCA Phase Ca ₂ (Fe, Ca) ₆ (Fe, Al, Si) ₆ O ₂₀ . 2019 , 105, 493-501		1
200	Thermal stability of Al ₂ MgC ₂ and thermodynamic modeling of the Al-Mg system - Application to grain refinement of Mg-Al alloys. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 67, 101678	1.9	2
199	Thermodynamic assessment of the Na ₂ O-Al ₂ O ₃ -SiO ₂ -B ₂ O ₃ pseudo-binary and -ternary systems. <i>Journal of Chemical Thermodynamics</i> , 2019 , 130, 251-268	2.9	11
198	Thermodynamic assessment and experimental investigation of the Al-Mn-Ni system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 64, 78-89	1.9	4
197	Bayesian uncertainty quantification and information fusion in CALPHAD-based thermodynamic modeling. <i>Acta Materialia</i> , 2019 , 164, 636-647	8.4	25

196	Thermodynamic assessment of the Co-Ta system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 64,	1.9	8
195	Emulation of short-range ordering within the Compound Energy Formalism: Application to the calcite-magnesite solid solution. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2019 , 64, 115-125	1.9	2
194	Thermodynamic and Experimental Evaluation of La _{1-x} Sr _x MnO ₃ Cathode in Presence of Cr-Containing Humidified Air. 2019 , 71, 3814-3824		2
193	Thermodynamic analysis of the topologically close packed β phase in the Co-Cr system. <i>Intermetallics</i> , 2019 , 105, 13-13	3.5	9
192	Analysis of formation and growth of the β phase in additively manufactured functionally graded materials. <i>Journal of Alloys and Compounds</i> , 2020 , 814, 151729	5.7	18
191	Thermodynamic modeling of the U ₃ O _{8-x} solid solution phase. 2020 , 530, 151844		3
190	Experimental Study and Thermodynamic Calculations of the Distribution of Ag, Au, Bi, and Zn Between Pb Metal and Pb ₂ Te ₃ Bi slag. 2020 , 6, 68-77		11
189	Thermodynamic modelling of the Ni ₂ Zr system. <i>Intermetallics</i> , 2020 , 116, 106640	3.5	4
188	Thermodynamic assessment of the CaO-Cu ₂ O-FeO-Fe ₂ O ₃ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 68, 101715	1.9	5
187	Thermodynamic reassessment of Fe-N and Fe-N-C systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 71, 102197	1.9	1
186	Computational thermodynamics and its applications. <i>Acta Materialia</i> , 2020 , 200, 745-792	8.4	36
185	Physical properties and solid-liquid equilibria for hexafluorophosphate-based ionic liquid ternary mixtures and their corresponding subsystems. 2020 , 316, 113742		2
184	Thermodynamic assessment of the Fe ₂ N ₂ O system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 71, 102213	1.9	5
183	Calphad Modeling of LRO and SRO Using ab initio Data. 2020 , 10, 998		2
182	A coherent set of model equations for various surface and interface energies in systems with liquid and solid metals and alloys. 2020 , 283, 102212		22
181	Computational Thermodynamic Calculations: FactSage from CALPHAD Thermodynamic Database to Virtual Process Simulation. 2020 , 51, 1851-1874		28
180	Critical evaluation and thermodynamic modeling of the Fe ₂ P and Fe ₃ P system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 70, 101795	1.9	3
179	Critical Evaluation and Thermodynamic Optimization of the Al-P and Fe-Al-P Systems. 2020 , 41, 598-614		0

178	The effect of cesium content on the thermodynamic stability and chemical durability of (Ba,Cs) _{1.33} (Al,Ti) ₈ O ₁₆ hollandite. 2020 , 103, 7310-7321		5
177	Thermodynamic modelling of the AlTiMn system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 71, 101793	1.9	3
176	Experimental study and thermodynamic optimization of the ZnO-FeO-Fe ₂ O ₃ -CaO-SiO ₂ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 71, 102011	1.9	4
175	Thermodynamic assessment of the NiCoCr system and Diffusion Study of its fcc phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 71, 101996	1.9	5
174	On the elaboration of the next generation of thermodynamic models of solid solutions. 2020 , 22, 19999-20013		
173	An improved method to evaluate the Joint Oxide-Gas Formation in (U,Pu)O ₂ irradiated fuels using the GERMINAL V2 code coupled to Calphad thermodynamic computations. 2020 , 6, 47		7
172	DFT-CEF Approach for the Thermodynamic Properties and Volume of Stable and Metastable AlNi Compounds. 2020 , 10, 1142		3
171	On the Application of the FactSage Thermochemical Software and Databases in Materials Science and Pyrometallurgy. 2020 , 8, 1156		2
170	Phase Equilibria and Minor Element Distributions in Complex Copper/Slag/Matte Systems. 2020 , 72, 3401-3409		7
169	Thermodynamic Database Development for the ZrO ₂ -MgO-MnOx System. 2020 , 41, 654-671		2
168	Critical Evaluation and Thermodynamic Optimization of the Fe-P System. 2020 , 51, 3108-3129		3
167	Critical evaluation and thermodynamic modeling of the PdSn system. <i>Intermetallics</i> , 2020 , 126, 106945	3.5	1
166	Modelling of short-range ordering kinetics in dilute multicomponent substitutional solid solutions. 2020 , 100, 1942-1961		
165	Asymptotic creep deformation behavior of modified HP steel after long-term service. 2020 , 34, 1997-2009		4
164	Viscosity of a Ternary Reciprocal System Consisting of 1-Alkylpyridinium Halides. 2020 , 59, 11823-11838		2
163	Computational thermochemistry of nuclear fuel. 2020 , 159-182		1
162	Thermodynamic modeling of G-phase and assessment of phase stabilities in reactor pressure vessel steels and cast duplex stainless steels. 2020 , 533, 152091		5
161	Determination of optimal compositions and properties for phase change materials in a solar electric generating station. 2020 , 210, 110506		4

160	Heat capacity measurement of $C14ZrMn2$ and thermodynamic re-assessment of the $MnZr$ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 68, 101745	1.9	5
159	Phase equilibria and thermodynamic assessment of the $MoNb-Re$ ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 70, 101797	1.9	1
158	Predicting the vibrational contribution to thermal and EOS properties of $Ni3X$ ($X=In,Sn$) intermetallic compounds. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 70, 101790	1.9	
157	Heat capacity measurements of the β phase $Mg2Zr4.2Ti0.8O12$ and thermodynamic modelling of the $ZrO2TiO2MgO$ system. <i>Journal of the European Ceramic Society</i> , 2020 , 40, 3304-3313	6	3
156	Non-stoichiometry Effects and Phase Equilibria in the Uranium-Carbon-Nitrogen Ternary System. 2020 , 51, 2549-2563		
155	Thermodynamic optimization of the $ZnOBeOBe2O3SiO2$ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 68, 101735	1.9	4
154	Diffusion-driven microstructure evolution in OpenCalphad. 2020 , 175, 109236		3
153	Structural stability of Co-V intermetallic phases and thermodynamic description of the Co-V system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2020 , 68, 101729-101729	1.9	2
152	Experimental Investigation of Phase Relations in the $ZrO2-La2O3-Yb2O3$ System. 2020 , 41, 311-328		6
151	Phase equilibria and multi-element interaction study in the metal-rich side of the $NbTiSiAl$ quaternary system. <i>Intermetallics</i> , 2020 , 120, 106760	3.5	3
150	Simulation of the chemical state of high burnup (U,Pu) $O2$ fuel in fast reactors based on thermodynamic calculations. 2020 , 532, 151969		11
149	Oxygen potential calculations for conventional and Cr-doped $UO2$ fuels based on solid solution thermodynamics. 2020 , 534, 152140		1
148	Controlling the crystallization of lithium borovanadate phases in an oxide glass composite using the CALPHAD approach. 2021 , 38, 1059-1070		
147	Formation of Nitride and Oxide Inclusions in Liquid Fe-Cr-Ti-Al Alloys. 2021 , 92, 2000508		1
146	Thermodynamic optimization of the MnB and $FeMnB$ systems. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 72, 102226	1.9	0
145	Laves phases: a review of their functional and structural applications and an improved fundamental understanding of stability and properties. 2021 , 56, 5321-5427		44
144	Uncertainty Quantification in Atomistic Modeling of Metals and Its Effect on Mesoscale and Continuum Modeling: A Review. 2021 , 73, 149		3
143	Design of hydrogen separatinwg Nb-Ti-Fe membranes with high permeability and low cost. 2021 , 257, 117945		6

142	CALPHAD as a powerful technique for design and fabrication of thermoelectric materials. 2021 , 9, 6634-6649	6
141	Air separation via two-step solar thermochemical cycles based on SrFeO and (Ba,La)SrFeO perovskite reduction/oxidation reactions to produce N: rate limiting mechanism(s) determination. 2021 , 23, 19280-19288	
140	Experimental Study and Thermodynamic Calculations in the CaO-Cu ₂ O-FeO-Fe ₂ O ₃ -SiO ₂ System for Applications in Novel Copper-Based Processes. 2021 , 7, 300-313	3
139	Experimental investigation and thermodynamic modeling of the Mg-Bi-Br ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 72, 102237	1.9 3
138	Equilibrium Distributions of Pb, Bi, and Ag between Fayalite Slag and Copper-Rich Metal, Calcium Ferrite Slag and Copper-Rich Metal. Thermodynamic Assessment and Experimental Study at 1250 °C. 2021 , 7, 569-582	4
137	Development of a Phase Field Tool Coupling With Thermodynamic Data for Microstructure Evolution Simulation of Alloys in Nuclear Reactors. 2021 , 8,	1
136	Data workflow to incorporate thermodynamic energies from Calphad databases into grand-potential-based phase-field models. 2021 , 56, 11932-11952	3
135	Phase Relations in the ZrO ₂ -MgO-FeO _x System: Experimental Data and Assessment of Thermodynamic Parameters. 2021 , 42, 254-277	0
134	Computational Assessment of Novel Predicted Compounds in Ni-Re Alloy System. 2021 , 42, 315-320	2
133	Derivations of Partial Molar Excess Gibbs Energy of Mixing Expressions for Common Thermodynamic Models. 2021 , 42, 333-347	1
132	Thermodynamic Modeling of the Fe-Mn-Ti System. 2021 , 42, 363-372	1
131	Thermodynamic assessment of the Co-Cr-Ni, Co-Cr-W and Co-Ni-W. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 73, 102252	1.9 2
130	An Insight from the CALPHAD Approach: How to Control the LaMnO ₃ Perovskite Formation Via the Molten Salt Synthesis. 2021 , 42, 419-427	1
129	Computational engineering of the oxygen electrode-electrolyte interface in solid oxide fuel cells. 2021 , 7,	0
128	T ₂ phase site occupancies in the Cr ₂ Si ₂ B system: a combined synchrotron-XRD/first-principles study. 2021 , 199, 113854	0
127	A sublattice phase-field model for direct CALPHAD database coupling. 2021 , 195, 110466	2
126	Development of Thermokinetic Tools for Phase Transformation Studies of Zr Alloys for Both In-Service and LOCA Conditions. 2021 , 833-854	
125	Thermodynamic Optimization of the Ternary Ga-Sn-Te System Using Modified Quasichemical Model. 2021 , 11, 1363	0

124	Tensile behavior of stainless steel 304L to Ni-20Cr functionally graded material: Experimental characterization and computational simulations. <i>Materialia</i> , 2021 , 18, 101151	3.2	3
123	Rapid screening of high-throughput ground state predictions. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 74, 102306	1.9	2
122	Thermodynamic modelling of the Al ₂ O ₃ -Fe system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 74, 102288	1.9	1
121	Effect of LCFeCr Alloy Additions on the Non-metallic Inclusion Characteristics in Ti-Containing Ferritic Stainless Steel. 1		2
120	Critical evaluation and thermodynamic modeling of the Ag-X (X=Mn, Y, Sr) binary systems. <i>Intermetallics</i> , 2021 , 136, 107260	3.5	1
119	Thermodynamic modelling of the ternary Bi-Ga-Te system for potential application in thermoelectric materials. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 74, 102326	1.9	3
118	The Thermodynamic Controls on Sulfide Saturation in Silicate Melts with Application to Ocean Floor Basalts. 2021 , 177-213		0
117	Thermodynamic modeling of the Al ₂ Nb ₃ system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 74, 102321	1.9	2
116	Air separation via a two-step solar thermochemical cycle based on (Ba,La) _x Sr _{1-x} FeO _{3-δ} Thermodynamic analysis. 2021 , 368, 115692		3
115	Phase Relationships in the Carbon-Titanium-Uranium System for Ultra-High Temperature Nuclear Fuels. 1		
114	Experimental investigation and thermodynamic modeling of the Mg ₂ Cu ₂ Ca ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 75, 102325	1.9	0
113	Critical assessment and thermodynamic modeling of the Al-Mn-O system. <i>Journal of Alloys and Compounds</i> , 2021 , 884, 161153	5.7	
112	Experimental measurement and thermodynamic evaluation of the Mg + Cu + Sr ternary system. <i>Journal of Chemical Thermodynamics</i> , 2021 , 163, 106582	2.9	1
111	Recent developments for molten salt systems in Thermochemica. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 75, 102341	1.9	2
110	Calculation of adsorption equilibria using CALPHAD models and software. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 75, 102323	1.9	
109	Experimental investigation and thermodynamic modeling of the ternary TiFe ₂ Mn system for hydrogen storage applications. <i>Journal of Alloys and Compounds</i> , 2022 , 891, 161957	5.7	1
108	The Development and Validation of a New Thermodynamic Database for Aluminium Alloys. 291-295		1
107	The Development and Validation of a New Thermodynamic Database for Ni-Based Alloys. 803-812		6

106	Development of a New Thermochemistry Solver for Multiphysics Simulations of Nuclear Materials. 2020 , 1013-1025		3
105	Impact of fission product inclusion on phase development in U3Si2 fuel. 2020 , 537, 152235		2
104	Review on the Phase Equilibria in Iron Ore Sinters. 2020 , 60, 2633-2648		8
103	Experimental measurement and thermodynamic model predictions of the distributions of Cu, As, Sb and Sn between liquid lead and PbOBeOBe2O3BiO2 slag. <i>International Journal of Materials Research</i> , 2020 , 111, 733-743	0.5	5
102	Alloy Gene Gibbs Energy Partition Function and Equilibrium Holographic Network Phase Diagrams of AuCu-Type Sublattice System. 2013 , 06, 415-442		5
101	pycalphad: CALPHAD-based Computational Thermodynamics in Python. 2017 , 5,		46
100	Notes on the creation and manipulation of solid solution models. 2021 , 176, 1		3
99	How high is the entropy in high entropy ceramics?. 2021 , 130, 150903		5
98	DFTTK: Density Functional Theory ToolKit for high-throughput lattice dynamics calculations. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 75, 102355	1.9	4
97	A thermodynamic assessment of the MgSnSb ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2021 , 75, 102361	1.9	1
96	Thermodynamic description of multi-component multi-phase alloys and its application to the solidification process. <i>International Journal of Materials Research</i> , 2008 , 99, 632-637	0.5	
95	The Development and Validation of a New Thermodynamic Database for Aluminum Alloys. 2012 , 291-295		
94	Calculation of the Phase Equilibria in Nb-Ni-Ti Ternary System. 361-370		
93	Thermodynamic Optimization of Mn-Si-C System. 2014 , 641-649		
92	The Application of a Recent Thermodynamic Model for Coke Crystallites: Chemisorption of Methyl Groups, Decomposition of Natural Gas, and the Reduction of Metal Oxides. 2015 , 331-338		
91	Alloy Gene Sequence Project and System Science Philosophy. 2017 , 10, 327-401		
90	Thermodynamic Modelling in the Frames of the TRIP-Matrix-Composite Development. 2020 , 621-649		
89	Computational Thermodynamics: Application to Nuclear Materials. 2020 , 814-849		

88	Thermodynamic Approach to the Development and Selection of Hardfacing Materials in Energy Industry. 2020 , 28, 84-89		2
87	Thermodynamics and Phase Equilibria of Iron-Base Systems. 2021 , 1-35		
86	Grand-potential based phase-field model for systems with interstitial sites. 2020 , 10, 22423		0
85	A structurally-consistent CASH+ sublattice solid solution model for fully hydrated C-S-H phases: Thermodynamic basis, methods, and Ca-Si-H ₂ O core sub-model. 2022 , 151, 106585		5
84	Thermodynamic Solution and Mixing Models: Non-electrolytes. 2020 , 283-317		
83	Thermodynamic Study on Solubility Products of Ti ₄ C ₂ S ₂ in Fe Using First-Principles Calculations. 2020 , 106, 911-923		
82	Thermodynamic Study on Solubility Products of Ti ₄ C ₂ S ₂ in Fe Using First-Principles Calculations. 2020 , 60, 745-755		
81	Thermodynamic and Structural Modelling of Non-Stoichiometric -Doped UO Solid Solutions = {La, Pr, Nd, Gd}. 2021 , 9, 705024		0
80	Site occupancy behavior of the binary β phase. 2021 , 122704		0
79	Thermodynamic Models of Multicomponent Nonstoichiometric Solution Phases Using Internal Process Order Parameters. <i>Acta Materialia</i> , 2021 , 223, 117462	8.4	1
78	Developments in Thermodynamic Models of Deposit-Induced Corrosion of High-Temperature Coatings. 2022 , 74, 260		0
77	Thermodynamic modeling of the Al-Co-Cr-Fe-Ni high entropy alloys supported by key experiments. <i>Journal of Alloys and Compounds</i> , 2021 , 897, 162722	5.7	1
76	Oxidation Mechanism During Pyrometallurgical Vanadium Extraction Process Using CO ₂ -Containing Gas. 1		
75	Fundamentals of solar thermochemical gas splitting materials. 2021 , 55-90		0
74	Binary TiBe system. Part II: Modelling of pressure-dependent phase stabilities. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022 , 76, 102383	1.9	2
73	Liquid Immiscibility and Thermodynamic Assessment of the Al ₂ O ₃ -TiO ₂ -Bi ₂ O ₃ System. 2022 , 43, 15		
72	Design of an additively manufactured functionally graded material of 316 stainless steel and Ti-6Al-4V with Ni-20Cr, Cr, and V intermediate compositions. 2022 , 51, 102649		1
71	Review of computational approaches to predict the thermodynamic stability of inorganic solids.		1

70	Phase equilibria of VCrMnFeCo high entropy alloys. <i>Journal of Alloys and Compounds</i> , 2022 , 903, 163950	5.7	1
69	Assessment of thermodynamic functions in the MgO-Al ₂ O ₃ -SiO ₂ system. <i>International Journal of Materials Research</i> , 2022 , 95, 793-805	0.5	2
68	Optimization of Thermochemical Stability of La-Based/Zr-Based Dual-Phase Composites for Oxygen Transport Membranes Via Computational Thermodynamics. <i>SSRN Electronic Journal</i> ,	1	
67	Making sustainable aluminum by recycling scrap: The science of dirty alloys. 2022 , 100947		8
66	Development of the Molten Salt Thermal Properties Database (MSTDBTC), example applications, and LiCl-KCl and UF ₃ -UF ₄ system assessments. 2022 , 563, 153631		1
65	Thermodynamic re-modelling of the Cu-Nb system: Integrating the nausite phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022 , 77, 102409	1.9	0
64	Experimental investigation and thermodynamic description of Mg-Sc-Zn ternary system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022 , 77, 102406	1.9	0
63	Thermodynamic Modeling and Mechanical Properties of Mg-Zn-(Y, Ce) Alloys: Review. <i>Crystals</i> , 2021 , 11, 1592	2.3	0
62	Thermodynamic Calculation of Fe-Ni and Fe-Ni-a Melting Diagrams at Pressures from 0.1 MPa to 7 GPa. <i>Progress in Physics of Metals</i> , 2021 , 22, 531-538	1.6	1
61	Theory of cross phenomena and their coefficients beyond Onsager theorem. <i>Materials Research Letters</i> , 2022 , 10, 393-439	7.4	2
60	Modified Calcium Manganites for Thermochemical Energy Storage Applications. <i>Frontiers in Energy Research</i> , 2022 , 10,	3.8	
59	Critical Evaluation and Thermodynamic Optimization of the Si-N, Si-C, C-N and Si-C-N Systems and Its Applications to High purity SiC Production. <i>Journal of the European Ceramic Society</i> , 2022 ,	6	0
58	Co-Based superalloy morphology evolution: A phase field study based on experimental thermodynamic and kinetic data. <i>Acta Materialia</i> , 2022 , 233, 117978	8.4	0
57	Thermodynamic description of high-pressure phase equilibria in the Fe-Ni system. <i>Journal of Alloys and Compounds</i> , 2022 , 914, 165304	5.7	
56	Thermodynamic modelling of the Ce-Ni system. <i>International Journal of Materials Research</i> , 2022 , 97, 737-743	0.5	
55	Experimental and thermodynamic evaluation of the Co-Cr system. <i>International Journal of Materials Research</i> , 2022 , 97, 1243-1250	0.5	
54	Thermodynamic assessment of the systems La ₂ O ₃ -Al ₂ O ₃ and La ₂ O ₃ -ZrO ₂ . <i>International Journal of Materials Research</i> , 2022 , 97, 1495-1501	0.5	1
53	Thermodynamic assessment of the Co-Ti-Be system and diffusion study of its fcc phase. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2022 , 77, 102430	1.9	0

- 52 Thermodynamic Modelling of the V-Ti-B System. *SSRN Electronic Journal*, 1
- 51 The metallic palladium-rhodium solution in interaction with oxygen: The Pd-Rh-O phase diagram and thermodynamics. *Journal of Chemical Thermodynamics*, **2022**, 172, 106831 2.9
- 50 New Approach to the Compound Energy Formalism (Nacef) Part Ii. Thermodynamic Modelling of the AlNiB System Supported by First-Principles Calculations. *SSRN Electronic Journal*, 1
- 49 Thermodynamic Calculations of the FeTiAl Melting Diagram in the Context of Gallium Nitride Crystallization under High Temperatures and Pressures. *Journal of Superhard Materials*, **2022**, 44, 73-78 0.9
- 48 Crystal chemistry and thermodynamic modelling of the Al₁₃(Fe,TM)₄ solid solutions (TM = Co, Cr, Ni, Pt). *Journal of Alloys and Compounds*, **2022**, 920, 165779 5.7 0
- 47 On the Thermodynamics and Phase Transformation Pathways in BCC-B2 Refractory Compositionally-Complex Superalloys. *SSRN Electronic Journal*, 1
- 46 Thermodynamic Modeling of Phase Equilibria in the NbZrNi System. *Inorganic Materials*, **2022**, 58, 509-515 0.9
- 45 Hydrogen-induced enhancement of thermal stability in VZr(H) metallic glasses. *Materialia*, **2022**, 101496 3.2 0
- 44 A thermodynamic model for high temperature corrosion applications: the (Na₂SO₄ + K₂SO₄ + ZnSO₄ + PbSO₄) system. *Chemical Engineering Science*, **2022**, 117847 4.4
- 43 Thermodynamic analysis of the AlNi system. *Intermetallics*, **2022**, 149, 107647 3.5
- 42 Computational modelling of the local structure and thermophysical properties of ternary MgCl₂-NaCl-KCl salt for thermal energy storage applications. *International Journal of Heat and Mass Transfer*, **2022**, 196, 123273 4.9
- 41 Integrated phase equilibria experimental study and thermodynamic modeling of the CrSiO, FeCrO and FeCrBiO systems. **2022**, 0
- 40 Critical Evaluation and Thermodynamic Optimization of the Cu-Zn, Cu-Se and Zn-Se Binary Systems. **2022**, 12, 1401
- 39 CALPHAD as a Toolbox to Facilitate the Development of HEAs.
- 38 Critical Evaluation and Thermodynamic Modeling of the Li-Se and Na-Se Binary Systems Using Combined CALPHAD and First-Principles Calculations Method. **2022**, 12, 1349
- 37 Assessment of the MgAlBb system supported by experiments and extrapolation to the MgAlBnBb quaternary system. **2022**, 78, 102460 0
- 36 Phase Equilibria of the Mg-Zn-Sm System in Mg-Rich Corner at 320 °C and 400 °C. **2022**, 12, 1553 1
- 35 A coupled experimental and thermodynamic assessment of the Mg-Bi-Sb and Zn-Bi-Sb ternary system and extrapolate to the Mg-Bi-Zn-Sb system. **2022**, 716, 179327 0

- 34 Thermodynamic modelling of the V₃Si system. **2022**, 79, 102477 ○
- 33 Energy landscapes in inorganic chemistry. **2022**, ○
- 32 Critical thermodynamic assessment of Mo₂C, Mo₃C, and Mo₄C systems, and its application to Mo carbo-nitride synthesis. ○
- 31 Modeling Short-Range Ordering in Binary BCC Ti-X (X = Nb, V, Zr) Alloys using CE-CVM. **2022**, 43, 511-526 ○
- 30 Development of a self-consistent thermodynamic database for Ga-In-Te system and experimental validation: a potential system for thermoelectric application. ○
- 29 The Oxidation Behavior of a Selection of South African Chromites. ○
- 28 Investigation on the microstructure, phase formation and properties of aluminium alloy coatings by stud spraying. **2022**, 33, 22256-22269 ○
- 27 Thermodynamic Assessments or Reassessments of 30 Pseudo-Binary and -Ternary Salt Systems. **2022**, 106931 ○
- 26 On the Thermodynamics and Phase Transformation Pathways in BCC-B2 Refractory Compositionally Complex Superalloys. ○
- 25 Thermodynamic Assessments of the Pd₃Ni and Pt₃Ni Systems With the Modified Quasi-chemical Model for Liquid. ○
- 24 Effects of basicity and Al₂O₃ content on the crystal structure of silico-ferrite of calcium and aluminum. **2022**, ○
- 23 Boriding of tungsten by the powder-pack process: Phase formation, growth kinetics and enhanced neutron shielding. **2023**, 110, 106049 ○
- 22 New approach to the compound energy formalism (NACEF) part I. Thermodynamic modeling based on the sublattice model. **2023**, 80, 102509 ○
- 21 Thermodynamic description of the Ti₃Ni₇O system. **2023**, 80, 102520 ○
- 20 The Al₅Fe₂ phase in the Al₂Fe system: The issue with the sublattice model. **2023**, 936, 168361 ○
- 19 Overcoming significant challenges in extracting off-stoichiometric thermodynamics using the compound energy formalism through complementary use of experimental and first principles data: A case study of Ba_{1-x}Sr_xFeO₃. **2023**, 390, 116115 ○
- 18 Thermodynamic description of Mg₂Ni₃Sn system supported by experimental work and extrapolation to the Mg₂Ni₃Al₃Sn quaternary system. **2023**, 80, 102525 ○
- 17 Thermodynamic modeling of the Mg₂Ni₃Sn ternary system with key experimental investigation. **2023**, 80, 102530 ○

- 16 Thermodynamic reassessment of Fe-Nb system. **2023**, 80, 102529 ○
- 15 New approach to the compound energy formalism (NACEF) Part II. Thermodynamic modelling of the Al-Nb system supported by first-principles calculations. **2023**, 80, 102522 ○
- 14 Computer Alloy Design of Ti Modified Al-Si-Mg-Sr Casting Alloys for Achieving Simultaneous Enhancement in Strength and Ductility. **2023**, 16, 306 2
- 13 Stabilization of Equiatomic Solutions Due to High-Entropy Effect. **2023**, ○
- 12 Experimental Investigation of Phase Relations and Thermodynamic Modelling of the Fe-Mn-Zr System. ○
- 11 Mg-Ti System up to 20 GPa: Its Phase Diagram and Stable Magnesium Carbides. **2023**, 127, 1965-1972 ○
- 10 A comprehensive study on the thermodynamics of the Al₁₃Fe₄ solid solution in the Al-Fe-Mn ternary system. **2023**, 944, 169054 ○
- 9 Shapes of phases in isothermal phase diagrams: what is wrong with the Thermo-Calc logo. ○
- 8 Experimental study and thermodynamic modeling of distribution of elements among slag, matte and metal in the Cu-Fe-O-Si-(Zn)(Al, Ca, Mg) system for copper slag cleaning applications. **2023**, 23, 5280-5300 ○
- 7 Thermodynamic assessment of the ternary Ni-Ti-Hf system. **2023**, 81, 102546 ○
- 6 Phase equilibria and defect chemistry of the La-Sr-Co-O system. **2023**, 43, 4419-4430 ○
- 5 Reactive metal additive manufacturing: Surface near Zr-Nb metallic glass composite formation and mechanical properties. **2023**, 66, 103457 ○
- 4 Phase Equilibria of the Cu-Se-Te Ternary System. ○
- 3 Pilling-Bedworth Ratio for Homogeneous Alloys: A Physically Sound Practical Generalization. ○
- 2 Modeling the diffusion-controlled phase transformations in transition metal carbide multilayer composites. **2023**, 101106 ○
- 1 Materials Design Directions for Solar Thermochemical Water Splitting. **2023**, 1-63 ○