Malin Selleby

List of Publications by Year
in descending order

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102 papers	2,821 citations	159358 30 h-index	197535 49 g-index
104 all docs	104 docs citations	104 times ranked	2182 citing authors

#	Article	IF	Citations
1	Phase Equilibria and Thermodynamic Properties in the Fe-Cr System. Critical Reviews in Solid State and Materials Sciences, 2010, 35, 125-152.	6.8	172
2	Calculations of thermophysical properties of cubic carbides and nitrides using the Debyeâ€“GrÃ¼neisen model. Acta Materialia, 2007, 55, 1215-1226.	3.8	155
3	Assessments of molar volume and thermal expansion for selected bcc, fcc and hcp metallic elements. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 68-89.	0.7	149
4	An improved thermodynamic modeling of the Feâ€“Cr system down to zero kelvin coupled with key experiments. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 355-366.	0.7	141
5	Theoretical modeling of molar volume and thermal expansion. Acta Materialia, 2005, 53, 2259-2272.	3.8	105
6	Thermodynamic Assessment of the CaO-Al2O3-SiO2 System. Journal of the American Ceramic Society, 2006, 89, 298-308.	1.9	105
7	Low-Density Steels: Complex Metallurgy for Automotive Applications. Jom, 2014, 66, 1747-1758.	0.9	86
8	Magnetic phase diagram of the Feâ€“Ni system. Acta Materialia, 2011, 59, 521-530.	3.8	73
9	Thermodynamics of stable and metastable structures in Feâ€“C system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 46, 148-158.	0.7	67
10	Thermodynamic reassessment of the Y 2O3â€“Al2O3â€“SiO2 system and its subsystems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 399-412.	0.7	61
11	Thermodynamic modelling of the Crâ€“Feâ€“Niâ€“O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 577-592.	0.7	58
12	Implementation of a new model for pressure dependence of condensed phases in Thermo-Calc. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2005, 29, 49-55.	0.7	57
13	Phase Equilibria and Thermodynamics in the Al2O3-SiO2 System-Modeling of Mullite and Liquid. Journal of the American Ceramic Society, 2005, 88, 2544-2551.	1.9	56
14	An assessment of the Ca-Fe-O system. Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science, 1990, 21, 2759-2776.	1.4	53
15	An improved magnetic model for thermodynamic modeling. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2012, 39, 11-20.	0.7	53
16	On the third-generation Calphad databases: An updated description of Mn. Physica Status Solidi (B): Basic Research, 2015, 252, 2199-2208.	0.7	52
17	Thermodynamic Assessment of the Fe-Mn-O System. Journal of Phase Equilibria and Diffusion, 2010, 31, 113-134.	0.5	50
18	Thermodynamic assessment of the MgOâ€“Al2O3â€“SiO2 system. Journal of Materials Research, 2005, 20, 975-986.	1.2	49

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19	Thermodynamic investigation of the galvanizing systems, I: Refinement of the thermodynamic description for the Feâ€“Zn system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 433-440.	0.7	44
20	A Critical Assessment of Tnermodynamic and Phase Diagram Data for the Al-O System. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 1992, 16, 173-179.	0.7	43
21	Thermodynamic analysis of the Ni-Ta system.. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 1994, 18, 99-107.	0.7	43
22	A re-evaluation of the liquid phases in the CaOâ€“Al2O3 and MgOâ€“Al2O3 systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2004, 28, 307-312.	0.7	43
23	Thermodynamic assessment of the Al-C-Fe system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 58, 34-49.	0.7	41
24	A reassessment of the Caî—¸Feî—¸O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 1996, 20, 381-392.	0.7	37
25	A thermodynamic re-assessment of Alâ€“V toward an assessment of the ternary Alâ€“Tiâ€“V system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 75-88.	0.7	36
26	The Alâ€“Feâ€“Mn system revisitedâ€”An updated thermodynamic description using the most recent binaries. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2013, 43, 86-93.	0.7	34
27	New description of metastable hcp phase for unaries Fe and Mn: Coupling between first-principles calculations and CALPHAD modeling. Physica Status Solidi (B): Basic Research, 2016, 253, 1830-1836.	0.7	34
28	PrecHiMn-4â€”A thermodynamic database for high-Mn steels. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 56, 49-57.	0.7	34
29	Modelling of acid and basic slags. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 1994, 18, 31-37.	0.7	32
30	Thermodynamic evaluation of pure Co for the third generation of thermodynamic databases. Physica Status Solidi (B): Basic Research, 2017, 254, 1600231.	0.7	32
31	Thermodynamic re-assessment of the Coâ€“Cr system supported by first-principles calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 52, 1-7.	0.7	31
32	A New Description of Pure C in Developing the Third Generation of Calphad Databases. Journal of Phase Equilibria and Diffusion, 2018, 39, 832-840.	0.5	29
33	An insight into using DFT data for Calphad modeling of solid phases in the third generation of Calphad databases, a case study for Al. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 65, 79-85.	0.7	29
34	The compound energy formalism: applications. Journal of Alloys and Compounds, 2001, 320, 177-188.	2.8	28
35	Parameters in the compound energy formalism for ionic systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 227-232.	0.7	28
36	Thermodynamic modelling of liquids: CALPHAD approaches and contributions from statistical physics. Physica Status Solidi (B): Basic Research, 2014, 251, 33-52.	0.7	28

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37	A thermodynamic assessment of the binary Fe-Mn system for the third generation of Calphad databases. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 64, 185-195.	0.7	26
38	An assessment of the Fe-O-Si system. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 1997, 28, 563-576.	1.0	25
39	Thermal expansion and compressibility of Co6W6C. Journal of Alloys and Compounds, 1999, 285, 242-245.	2.8	25
40	An assessment of the Ca-Fe-O-Si system. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 1997, 28, 577-596.	1.0	24
41	Thermodynamic assessment of the Crâ€“Mnâ€“O system. Journal of Alloys and Compounds, 2010, 507, 84-92.	2.8	24
42	A thermodynamic database for special brass. Journal of Phase Equilibria and Diffusion, 2003, 24, 110-121.	0.3	23
43	Effect of vacuum degassing on non-metallic inclusions in an ASEA-SKF ladle furnace. Ironmaking and Steelmaking, 2013, 40, 470-477.	1.1	22
44	Thermodynamic calculations and experimental verification in the WCâ€“Coâ€“Cr cemented carbide system. International Journal of Refractory Metals and Hard Materials, 2015, 48, 257-262.	1.7	21
45	Thermodynamic investigation of the Al-Fe-Mn system over the whole composition and wide temperature ranges. Journal of Alloys and Compounds, 2018, 742, 1046-1057.	2.8	21
46	Thermodynamic reassessment of the Si3N4â€“AlNâ€“Al2O3â€“SiO2 systemâ€”Modeling of the SiAlON and liquid phases. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2007, 31, 269-280.	0.7	19
47	Thermodynamic assessment of the Vâ€“O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 144-160.	0.7	19
48	A method for handling the extrapolation of solid crystalline phases to temperatures far above their melting point. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2020, 68, 101737.	0.7	19
49	Thermodynamic assessment of the Niâ€“Te system. Journal of Materials Science, 2019, 54, 11304-11319.	1.7	18
50	Thermodynamic assessment of the Mnâ€“S and Feâ€“Mnâ€“S systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 48, 95-105.	0.7	17
51	Thermodynamic analysis of the Wâ€“Coâ€“Cr system supported by ab initio calculations and verified with quaternary data. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 50, 59-67.	0.7	15
52	Point defects in B2 compounds. Journal of Alloys and Compounds, 2001, 329, 208-213.	2.8	14
53	Investigation of Spinodal Decomposition in Fe-Cr Alloys: CALPHAD Modeling and Phase Field Simulation. Solid State Phenomena, 0, 172-174, 1060-1065.	0.3	14
54	Evaluation of austenite reformation in duplex stainless steel weld metal using computational thermodynamics. Welding in the World, Le Soudage Dans Le Monde, 2014, 58, 217-224.	1.3	14

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55	Ab-initio based search for late blooming phase compositions in iron alloys. Journal of Nuclear Materials, 2018, 509, 225-236.	1.3	14
56	Thermodynamic assessment of the Fe-Te system. Part II: Thermodynamic modeling. Journal of Alloys and Compounds, 2018, 767, 883-893.	2.8	13
57	Thermodynamic analysis of the Coâ€“Crâ€“C system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 46, 226-236.	0.7	12
58	Ordering in ternary BCC alloys applied to the Alâ€“Feâ€“Mn system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2015, 51, 211-219.	0.7	12
59	The third generation Calphad description of Alâ€“C including revisions of pure Al and C. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 72, 102250.	0.7	12
60	Adding C to the thermodynamic description of the Crâ€“Feâ€“Niâ€“O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2009, 33, 393-397.	0.7	11
61	Thermodynamic Assessment of the Fe-Ca-S, Fe-Mg-O and Fe-Mg-S Systems. Journal of Phase Equilibria and Diffusion, 2016, 37, 277-292.	0.5	11
62	A new thermodynamic description of stable Cr-carbides for the third generation of thermodynamic database. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 59, 107-111.	0.7	11
63	Thermodynamic modeling of the Al-C-Mn system supported by ab initio calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 60, 222-230.	0.7	11
64	Trapping of vacancies by rapid solidification. Acta Materialia, 2002, 50, 3285-3293.	3.8	10
65	Microstructure and mechanical properties of spray formed ultrahigh-carbon steels. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 383, 45-49.	2.6	10
66	An assessment of the Ti-V-O system. Journal of Alloys and Compounds, 2017, 722, 365-374.	2.8	10
67	An assessment of the Ca-V-O system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 56, 29-40.	0.7	10
68	An attempt to correct the quasichemical model. Acta Materialia, 2009, 57, 5237-5244.	3.8	9
69	Thermodynamic assessment of the Mnâ€“Niâ€“O system. International Journal of Materials Research, 2010, 101, 1222-1231.	0.1	9
70	Oxygen Activity Calculations of Molten Steel: Comparison With Measured Results. Steel Research International, 2013, 84, 136-145.	1.0	8
71	The Effect of Oxygen Potential on the Sulfide Capacity for Slags Containing Multivalent Species. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2016, 47, 3039-3045.	1.0	8
72	Thermodynamic Modeling of Pure Co Accounting Two Magnetic States for the Fcc Phase. Journal of Phase Equilibria and Diffusion, 2018, 39, 502-509.	0.5	8

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73	A reassessment of the non-stoichiometry of fayalite. Physics and Chemistry of Minerals, 1996, 23, 387.	0.3	7
74	Atomic, Electronic, and Magnetic Structure of Iron-Based Sigma-Phases. Materials Research Society Symposia Proceedings, 2004, 842, 185.	0.1	7
75	Thermodynamic investigations of the C-Cr-Fe system by galvanic cell technique. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2005, 36, 263-270.	1.0	7
76	Experimental Determination of the Solubility of Co in the Cr-Based Carbides Cr23C6, Cr7C3, and Cr3C2. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2014, 45, 4820-4828.	1.1	7
77	Prediction of Martensite Start Temperature for Lightweight Fe-Mn-Al-C Steels. Journal of Phase Equilibria and Diffusion, 2018, 39, 476-489.	0.5	7
78	CALPHAD: Method for calculation of finite temperature thermodynamic properties for magnetic allotropesâ€"Case study on Fe, Co and Ni. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102320.	0.7	7
79	The effect of copper on secondary phase precipitation in duplex stainless steel â€“ a thermodynamic calculations approach. International Journal of Materials Research, 2005, 96, 918-923.	0.8	6
80	A third generation Calphad description of pure W. Materials Chemistry and Physics, 2022, 276, 125445.	2.0	6
81	The sharpness of melting maxima. Journal of Phase Equilibria and Diffusion, 1999, 20, 288-294.	0.3	5
82	Use of chemical potential of a compound in potential phase diagrams. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 342-345.	0.7	4
83	Process-time Optimization of Vacuum Degassing Using a Genetic Alloy Design Approach. Materials, 2014, 7, 7997-8011.	1.3	4
84	Reprint of â€œThermodynamic calculations and experimental verification in the WCâ€“Coâ€“Cr cemented carbide systemâ€• International Journal of Refractory Metals and Hard Materials, 2015, 49, 400-405.	1.7	4
85	Methods for storage of Gibbs energy data of substances. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 53, 146-150.	0.7	4
86	Thermodynamic description of the Fe-Ca-O-S system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 57, 118-125.	0.7	4
87	Experimental study of carbides in the Tiâ€“Crâ€“C system. Journal of Materials Science, 2019, 54, 12358-12370.	1.7	4
88	A Third Generation Calphad Description of Fe: Revisions of Fcc, Hcp and Liquid. Journal of Phase Equilibria and Diffusion, 2022, 43, 287-303.	0.5	4
89	Discussion of cementite layer formation and sooting. Scripta Materialia, 2010, 63, 1037-1040.	2.6	2
90	Comparison between measured CaO and Al₂O₃normalised to CaOâ€“Al₂O₃in top slag, calcium aluminate inclusions and results of theoretical calculations. Ironmaking and Steelmaking, 2013, 40, 369-375.	1.1	2

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91	Improving Steel and Steelmakingâ€"an Ionic Liquid Database for Alloy Process Design. Integrating Materials and Manufacturing Innovation, 2018, 7, 195-201.	1.2	2
92	End-member compounds of a 4-sublattice model of multicomponent BCC solid solutions. Data in Brief, 2018, 20, 1018-1022.	0.5	2
93	Calphad Modeling of LRO and SRO Using ab initio Data. Metals, 2020, 10, 998.	1.0	2
94	Precision Thermal Treatments, Atom Probe Characterization, and Modeling to Describe the Fe-Cr Metastable Miscibility Gap. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2021, 52, 1453-1464.	1.1	2
95	3D Analysis of Phase Separation in Ferritic Stainless Steels. , 2012, , 221-226.		2
96	Thermodynamic assessment and binary nucleation modeling of Sn-seeded InGaAs nanowires. Journal of Crystal Growth, 2017, 478, 152-158.	0.7	1
97	A third generation Calphad description of Wâ€"C including a revision of liquid C. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 78, 102449.	0.7	1
98	Computational thermodynamics as tool to study microstructural evolution of EAF duplex stainless steelmaking slags. Ironmaking and Steelmaking, 2012, 39, 51-58.	1.1	0
99	Thermodynamic assessment of the Feâ€"Niâ€"Te system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 67, 101672.	0.7	0
100	Adiabatic and quasi-adiabatic transformations. , 2008, , 263-266.		0
101	3D Analysis of Phase Separation in Ferritic Stainless Steels. , 0, , 221-226.		0
102	Thermodynamic assessment of the C Cr Ti systemâ€"Supported by DFT calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102405.	0.7	0