Fritz KÃ¶rmann

List of Publications by Year
in descending order

75 papers	4,486 citations	87723 38 h-index	102304 66 g-index
78 all docs	78 docs citations	78 times ranked	3146 citing authors

#	Article	IF	Citations
1	Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one. Acta Materialia, 2015, 100, 90-97.	3.8	389
2	Ultrastrong Mediumâ€Entropy Singleâ€Phase Alloys Designed via Severe Lattice Distortion. Advanced Materials, 2019, 31, e1807142.	11.1	301
3	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
4	Ab initio phase stabilities and mechanical properties of multicomponent alloys: A comprehensive review for high entropy alloys and compositionally complex alloys. Materials Characterization, 2019, 147, 464-511.	1.9	231
5	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
6	Engineering atomic-level complexity in high-entropy and complex concentrated alloys. Nature Communications, 2019, 10, 2090.	5.8	182
7	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157
8	Lattice Distortions in the FeCoNiCrMn High Entropy Alloy Studied by Theory and Experiment. Entropy, 2016, 18, 321.	1.1	151
9	Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials. Npj Computational Materials, 2019, 5, .	3.5	110
10	Phonon broadening in high entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	100
11	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
12	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93
13	Long-ranged interactions in bcc NbMoTaW high-entropy alloys. Materials Research Letters, 2017, 5, 35-40.	4.1	86
14	â€œTreasure mapsâ€•for magnetic high-entropy-alloys from theory and experiment. Applied Physics Letters, 2015, 107, .	1.5	84
15	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
16	Dislocation-induced breakthrough of strength and ductility trade-off in a non-equiatomic high-entropy alloy. Acta Materialia, 2020, 185, 45-54.	3.8	76
17	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
18	Lambda transitions in materials science: Recent advances in CALPHAD and firstâ€principles modelling. Physica Status Solidi (B): Basic Research, 2014, 251, 53-80.	0.7	75

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19	Thermodynamic properties of cementite (). Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 129-133.	0.7	72
20	Computationally-driven engineering of sublattice ordering in a hexagonal AlHfScTiZr high entropy alloy. Scientific Reports, 2017, 7, 2209.	1.6	71
21	Accurate electronic free energies of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi mathvariant="italic">d</mml:mi><mml:mo>,</mml:mo><mml:mn>4</mml:mn><mml:mi mathvariant="italic">d</mml:mi></mml:mrow></mml:math> , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>5</mml:mn><mml:mi mathvariant="italic">d</mml:mi></mml:mrow></mml:math> transition metals at high temperatures.	1.1	70
22	Shear band-driven precipitate dispersion for ultrastrong ductile medium-entropy alloys. Nature Communications, 2021, 12, 4703.	5.8	70
23	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. Entropy, 2018, 20, 655.	1.1	69
24	Interplay between Lattice Distortions, Vibrations and Phase Stability in NbMoTaW High Entropy Alloys. Entropy, 2016, 18, 403.	1.1	63
25	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
26	Rescaled Monte Carlo approach for magnetic systems:Ab initiothermodynamics of bcc iron. Physical Review B, 2010, 81, .	1.1	57
27	Ab initiobased determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. Physical Review B, 2011, 84, .	1.1	57
28	Operando Phonon Studies of the Protonation Mechanism in Highly Active Hydrogen Evolution Reaction Pentlandite Catalysts. Journal of the American Chemical Society, 2017, 139, 14360-14363.	6.6	53
29	Anomalous Phonon Lifetime Shortening in Paramagnetic CrN Caused by Spin-Lattice Coupling: A Combined Spin and AbÂInitio Molecular Dynamics Study. Physical Review Letters, 2018, 121, 125902.	2.9	53
30	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	3.5	52
31	Beyond Solid Solution Highâ€Entropy Alloys: Tailoring Magnetic Properties via Spinodal Decomposition. Advanced Functional Materials, 2021, 31, 2007668.	7.8	51
32	Pressure dependence of the Curie temperature in bcc iron studied byab initiosimulations. Physical Review B, 2009, 79, .	1.1	49
33	Effects of Cr/Ni ratio on physical properties of Cr-Mn-Fe-Co-Ni high-entropy alloys. Acta Materialia, 2022, 227, 117693.	3.8	47
34	Surface segregation in Cr-Mn-Fe-Co-Ni high entropy alloys. Applied Surface Science, 2020, 533, 147471.	3.1	46
35	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. Physical Review B, 2011, 83, .	1.1	45
36	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45

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37	Strong impact of lattice vibrations on electronic and magnetic properties of paramagnetic Fe revealed by disordered local moments molecular dynamics. Physical Review B, 2016, 93, .	1.1	43
38	Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128, .	1.1	40
39	Effects of cryogenic temperature on tensile and impact properties in a medium-entropy VCoNi alloy. Journal of Materials Science and Technology, 2021, 90, 159-167.	5.6	36
40	Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. Intermetallics, 2019, 111, 106520.	1.8	34
41	Influence of magnetic excitations on the phase stability of metals and steels. Current Opinion in Solid State and Materials Science, 2016, 20, 77-84.	5.6	31
42	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. Physical Review Materials, 2019, 3, .	0.9	30
43	Effect of solid-solution strengthening on deformation mechanisms and strain hardening in medium-entropy V1-Cr CoNi alloys. Journal of Materials Science and Technology, 2022, 108, 270-280.	5.6	30
44	Determining the Elasticity of Materials Employing Quantumâ€mechanical Approaches: From the Electronic Ground State to the Limits of Materials Stability. Steel Research International, 2011, 82, 86-100.	1.0	27
45	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	0.9	24
46	Element-resolved local lattice distortion in complex concentrated alloys: An observable signature of electronic effects. Acta Materialia, 2021, 216, 117135.	3.8	22
47	Design of a dual-phase hcp-bcc high entropy alloy strengthened by ï‰ nanoprecipitates in the Sc-Ti-Zr-Hf-Re system. Materials and Design, 2020, 192, 108716.	3.3	20
48	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	19
49	Thermodynamic modeling of chromium: strong and weak magnetic coupling. Journal of Physics Condensed Matter, 2013, 25, 425401.	0.7	18
50	Combined Al and C alloying enables mechanism-oriented design of multi-principal element alloys: Ab initio calculations and experiments. Scripta Materialia, 2020, 178, 366-371.	2.6	18
51	A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065.	1.4	18
52	Hidden Effects of Negative Stacking Fault Energies in Complex Concentrated Alloys. Physical Review Letters, 2021, 126, 255502.	2.9	18
53	Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. Physical Review Materials, 2019, 3, .	0.9	18
54	Unveiling the mechanism of abnormal magnetic behavior of FeNiCoMnCu high-entropy alloys through a joint experimental-theoretical study. Physical Review Materials, 2020, 4, .	0.9	18

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55	Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. Physical Review Materials, 2020, 4, .	0.9	18
56	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. Acta Materialia, 2016, 102, 241-250.	3.8	17
57	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	3.5	17
58	Correlation analysis of strongly fluctuating atomic volumes, charges, and stresses in body-centered cubic refractory high-entropy alloys. Physical Review Materials, 2020, 4, .	0.9	17
59	Influence of the dislocation core on the glide of the Â½ã€ˆ111ã€‰{110} edge dislocation in bcc-iron: An embedded atom method study. Computational Materials Science, 2014, 87, 274-282.	1.4	16
60	Thermodynamics up to the melting point in a TaVCrW high entropy alloy: Systematic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>a</mml:mi><mml:mi>b</mml:mi></mml:mrow><mml:mo study aided by machine learning potentials. Physical Review B, 2022, 105, .	1.1	16
61	Impact of magnetic fluctuations on lattice excitations in fcc nickel. Journal of Physics Condensed Matter, 2016, 28, 076002.	0.7	15
62	Performance of the standard exchange-correlation functionals in predicting melting properties fully from first principles: Application to Al and magnetic Ni. Physical Review B, 2020, 101, .	1.1	15
63	Atomistic Modelingâ€Based Design of Novel Materials. Advanced Engineering Materials, 2017, 19, 1600688.	1.6	14
64	Impact of Co and Fe Doping on the Martensitic Transformation and the Magnetic Properties in Niâ€Mnâ€Based Heusler Alloys. Physica Status Solidi (B): Basic Research, 2018, 255, 1700455.	0.7	14
65	B2 ordering in body-centered-cubic AlNbTiV refractory high-entropy alloys. Physical Review Materials, 2021, 5, .	0.9	14
66	Quaternary Al-Cu-Mg-Si Q Phase: Sample Preparation, Heat Capacity Measurement and First-Principles Calculations. Journal of Phase Equilibria and Diffusion, 2016, 37, 119-126.	0.5	12
67	Green function theory versus quantum Monte Carlo calculations for thin magnetic films. Physical Review B, 2007, 75, .	1.1	9
68	Reliability evaluation of thermophysical properties from first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 335401.	0.7	9
69	Finite-temperature interplay of structural stability, chemical complexity, and elastic properties of bcc multicomponent alloys from ab initio trained machine-learning potentials. Physical Review Materials, 2021, 5, .	0.9	9
70	Phonons in magnetically disordered materials: Magnetic versus phononic time scales. Physical Review B, 2020, 101, .	1.1	8
71	Impact of N on the Stacking Fault Energy and Phase Stability of FCC CrMnFeCoNi: An Ab Initio Study. Journal of Phase Equilibria and Diffusion, 2021, 42, 551-560.	0.5	7
72	A new type of temperature driven reorientation transition in magnetic thin films. European Physical Journal B, 2006, 53, 463-469.	0.6	3

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73	Design of compositionally complex catalysts: Role of surface segregation. Journal of Materials Research and Technology, 2021, 14, 1830-1836.	2.6	3
74	Iron-rich High Entropy Alloys. , 2021, , 389-421.		1
75	Cu cap layer on Ni8/Cu(001): reorientation and TC-shift. European Physical Journal B, 2008, 65, 499-504.	0.6	0