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	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
2	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
3	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	3.5	52
4	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, .	3.5	26
5	Beyond Solid Solution Highâ€Entropy Alloys: Tailoring Magnetic Properties via Spinodal Decomposition. Advanced Functional Materials, 2021, 31, 2007668.	7.8	51
6	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	3.5	17
7	A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065.	1.4	18
8	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
9	B2 ordering in body-centered-cubic AlNbTiV refractory high-entropy alloys. Physical Review Materials, 2021, 5, .	0.9	14
10	Hidden Effects of Negative Stacking Fault Energies in Complex Concentrated Alloys. Physical Review Letters, 2021, 126, 255502.	2.9	18
11	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
12	Shear band-driven precipitate dispersion for ultrastrong ductile medium-entropy alloys. Nature Communications, 2021, 12, 4703.	5.8	70
13	Element-resolved local lattice distortion in complex concentrated alloys: An observable signature of electronic effects. Acta Materialia, 2021, 216, 117135.	3.8	22
14	Design of compositionally complex catalysts: Role of surface segregation. Journal of Materials Research and Technology, 2021, 14, 1830-1836.	2.6	3
15	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
16	Iron-rich High Entropy Alloys. , 2021, , 389-421.		1
17	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
18	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

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19	Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128, .	1.1	40
20	Surface segregation in Cr-Mn-Fe-Co-Ni high entropy alloys. Applied Surface Science, 2020, 533, 147471.	3.1	46
21	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
22	Phonons in magnetically disordered materials: Magnetic versus phononic time scales. Physical Review B, 2020, 101, .	1.1	8
23	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
24	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
25	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
26	Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. Physical Review Materials, 2020, 4, .	0.9	18
27	Short-range order in face-centered cubic VCoNi alloys. Physical Review Materials, 2020, 4, .	0.9	24
28	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
29	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
30	Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. Intermetallics, 2019, 111, 106520.	1.8	34
31	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
32	Engineering atomic-level complexity in high-entropy and complex concentrated alloys. Nature Communications, 2019, 10, 2090.	5.8	182
33	Ultrastrong Mediumâ€Entropy Singleâ€Phase Alloys Designed via Severe Lattice Distortion. Advanced Materials, 2019, 31, e1807142.	11.1	301
34	Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. Physical Review Materials, 2019, 3, .	0.9	18
35	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
36	Temperature-dependent phonon spectra of magnetic random solid solutions. Npj Computational Materials, 2018, 4, .	3.5	19

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37	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
38	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
39	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
40	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
41	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45
42	Atomistic Modelingâ€Based Design of Novel Materials. Advanced Engineering Materials, 2017, 19, 1600688.	1.6	14
43	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
44	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. Ph	1.1	70
45	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
46	Computationally-driven engineering of sublattice ordering in a hexagonal AlHfScTiZr high entropy alloy. Scientific Reports, 2017, 7, 2209.	1.6	71
47	Long-ranged interactions in bcc NbMoTaW high-entropy alloys. Materials Research Letters, 2017, 5, 35-40.	4.1	86
48	Phonon broadening in high entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	100
49	Interplay between Lattice Distortions, Vibrations and Phase Stability in NbMoTaW High Entropy Alloys. Entropy, 2016, 18, 403.	1.1	63
50	Lattice Distortions in the FeCoNiCrMn High Entropy Alloy Studied by Theory and Experiment. Entropy, 2016, 18, 321.	1.1	151
51	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
52	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
53	Impact of magnetic fluctuations on lattice excitations in fcc nickel. Journal of Physics Condensed Matter, 2016, 28, 076002.	0.7	15
54	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

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55	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. Acta Materialia, 2016, 102, 241-250.	3.8	17
56	â€œTreasure mapsâ€•for magnetic high-entropy-alloys from theory and experiment. Applied Physics Letters, 2015, 107, .	1.5	84
57	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
58	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
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	Reliability evaluation of thermophysical properties from first-principles calculations. Journal of Physics Condensed Matter, 2014, 26, 335401.	0.7	9
61	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93
62	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
63	Thermodynamic modeling of chromium: strong and weak magnetic coupling. Journal of Physics Condensed Matter, 2013, 25, 425401.	0.7	18
64	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
65	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157
66	Ab initiobased determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. Physical Review B, 2011, 84, .	1.1	57
67	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
68	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. Physical Review B, 2011, 83, .	1.1	45
69	Rescaled Monte Carlo approach for magnetic systems:Ab initiothermodynamics of bcc iron. Physical Review B, 2010, 81, .	1.1	57
70	Thermodynamic properties of cementite (). Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2010, 34, 129-133.	0.7	72
71	Pressure dependence of the Curie temperature in bcc iron studied byab initiosimulations. Physical Review B, 2009, 79, .	1.1	49
72	Cu cap layer on Ni8/Cu(001): reorientation and TC-shift. European Physical Journal B, 2008, 65, 499-504.	0.6	0

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73	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
74	Green function theory versus quantum Monte Carlo calculations for thin magnetic films. Physical Review B, 2007, 75, .	1.1	9
75	A new type of temperature driven reorientation transition in magnetic thin films. European Physical Journal B, 2006, 53, 463-469.	0.6	3