Fritz Krmann

List of Publications by Citations

74 papers	2,779 citations	30 h-index	51 g-index
77 ext. papers	3,652 ext. citations	5.6 avg, IF	5.69 L-index

#	Paper	IF	Citations
74	Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one. *Acta Materialia*, **2015**, 100, 90-97	8.4	277
73	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. *Acta Materialia*, **2017**, 136, 262-270	8.4	179
72	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	3.9	152
71	Free energy of bcc iron: Integrated ab initio derivation of vibrational, electronic, and magnetic contributions. *Physical Review B*, **2008**, 78,	3.3	152
70	Ultrastrong Medium-Entropy Single-Phase Alloys Designed via Severe Lattice Distortion. *Advanced Materials*, **2019**, 31, e1807142	24	132
69	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. *Physical Review B*, **2012**, 85,	3.3	114
68	Engineering atomic-level complexity in high-entropy and complex concentrated alloys. *Nature Communications*, **2019**, 10, 2090	17.4	102
67	Lattice Distortions in the FeCoNiCrMn High Entropy Alloy Studied by Theory and Experiment. *Entropy*, **2016**, 18, 321	2.8	100
66	Structural stability and thermodynamics of CrN magnetic phases from ab initio calculations and experiment. *Physical Review B*, **2014**, 90,	3.3	78
65	Temperature dependent magnon-phonon coupling in bcc Fe from theory and experiment. *Physical Review Letters*, **2014**, 113, 165503	7.4	68
64	Treasure maps for magnetic high-entropy-alloys from theory and experiment. *Applied Physics Letters*, **2015**, 107, 142404	3.4	68
63	Advancing density functional theory to finite temperatures: methods and applications in steel design. *Journal of Physics Condensed Matter*, **2012**, 24, 053202	1.8	66
62	Thermodynamic properties of cementite (Fe3C). *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, **2010**, 34, 129-133	1.9	64
61	Lambda transitions in materials science: Recent advances in CALPHAD and first-principles modelling. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 53-80	1.3	62
60	Long-ranged interactions in bcc NbMoTaW high-entropy alloys. *Materials Research Letters*, **2017**, 5, 35-40	7.4	62
59	Phonon broadening in high entropy alloys. *Npj Computational Materials*, **2017**, 3,	10.9	61
58	Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials. *Npj Computational Materials*, **2019**, 5,	10.9	60

57	Rescaled Monte Carlo approach for magnetic systems: Ab initio thermodynamics of bcc iron. *Physical Review B*, **2010**, 81,	3.3	51
56	Ab initio based determination of thermodynamic properties of cementite including vibronic, magnetic, and electronic excitations. *Physical Review B*, **2011**, 84,	3.3	50
55	Accurate electronic free energies of the 3d,4d, and 5d transition metals at high temperatures. *Physical Review B*, **2017**, 95,	3.3	46
54	Computationally-driven engineering of sublattice ordering in a hexagonal AlHfScTiZr high entropy alloy. *Scientific Reports*, **2017**, 7, 2209	4.9	46
53	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. *Npj Computational Materials*, **2019**, 5,	10.9	44
52	Pressure dependence of the Curie temperature in bcc iron studied by ab initio simulations. *Physical Review B*, **2009**, 79,	3.3	44
51	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	16.4	42
50	Impact of Chemical Fluctuations on Stacking Fault Energies of CrCoNi and CrMnFeCoNi High Entropy Alloys from First Principles. *Entropy*, **2018**, 20,	2.8	42
49	Interplay between Lattice Distortions, Vibrations and Phase Stability in NbMoTaW High Entropy Alloys. *Entropy*, **2016**, 18, 403	2.8	40
48	Dislocation-induced breakthrough of strength and ductility trade-off in a non-equiatomic high-entropy alloy. *Acta Materialia*, **2020**, 185, 45-54	8.4	38
47	Role of spin quantization in determining the thermodynamic properties of magnetic transition metals. *Physical Review B*, **2011**, 83,	3.3	36
46	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. *Physical Review B*, **2018**, 98,	3.3	33
45	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,	3.3	31
44	Determining the Elasticity of Materials Employing Quantum-mechanical Approaches: From the Electronic Ground State to the Limits of Materials Stability. *Steel Research International*, **2011**, 82, 86-100	1.6	26
43	Anomalous Phonon Lifetime Shortening in Paramagnetic CrN Caused by Spin-Lattice Coupling: A Combined Spin and Ab□nitio Molecular Dynamics Study. *Physical Review Letters*, **2018**, 121, 125902	7.4	25
42	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. *Physical Review B*, **2018**, 97,	3.3	23
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	12	21
40	Impact of interstitial C on phase stability and stacking-fault energy of the CrMnFeCoNi high-entropy alloy. *Physical Review Materials*, **2019**, 3,	3.2	21

39	Surface segregation in Cr-Mn-Fe-Co-Ni high entropy alloys. *Applied Surface Science*, **2020**, 533, 147471	6.7	21
38	Beyond Solid Solution High-Entropy Alloys: Tailoring Magnetic Properties via Spinodal Decomposition. *Advanced Functional Materials*, **2021**, 31, 2007668	15.6	21
37	Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. *Intermetallics*, **2019**, 111, 106520	3.5	17
36	Frontiers in atomistic simulations of high entropy alloys. *Journal of Applied Physics*, **2020**, 128, 150901	2.5	16
35	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. *Acta Materialia*, **2016**, 102, 241-250	8.4	15
34	Correlation analysis of strongly fluctuating atomic volumes, charges, and stresses in body-centered cubic refractory high-entropy alloys. *Physical Review Materials*, **2020**, 4,	3.2	14
33	Temperature-dependent phonon spectra of magnetic random solid solutions. *Npj Computational Materials*, **2018**, 4,	10.9	13
32	Impact of magnetic fluctuations on lattice excitations in fcc nickel. *Journal of Physics Condensed Matter*, **2016**, 28, 076002	1.8	13
31	Thermodynamic modeling of chromium: strong and weak magnetic coupling. *Journal of Physics Condensed Matter*, **2013**, 25, 425401	1.8	12
30	Impact of Co and Fe Doping on the Martensitic Transformation and the Magnetic Properties in Ni-Mn-Based Heusler Alloys. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1700455	1.3	12
29	Influence of the dislocation core on the glide of the <1 1 1>{1 1 0} edge dislocation in bcc-iron: An embedded atom method study. *Computational Materials Science*, **2014**, 87, 274-282	3.2	11
28	Unveiling the mechanism of abnormal magnetic behavior of FeNiCoMnCu high-entropy alloys through a joint experimental-theoretical study. *Physical Review Materials*, **2020**, 4,	3.2	11
27	Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. *Physical Review Materials*, **2020**, 4,	3.2	11
26	Atomistic Modeling-Based Design of Novel Materials . *Advanced Engineering Materials*, **2017**, 19, 1600688	3.5	10
25	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	5.6	10
24	Design of a dual-phase hcp-bcc high entropy alloy strengthened by nanoprecipitates in the Sc-Ti-Zr-Hf-Re system. *Materials and Design*, **2020**, 192, 108716	8.1	9
23	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	1	9
22	Green function theory versus quantum Monte Carlo calculations for thin magnetic films. *Physical Review B*, **2007**, 75,	3.3	9

21	Ab initio phase stabilities of Ce-based hard magnetic materials and comparison with experimental phase diagrams. *Physical Review Materials*, **2019**, 3,	3.2	9
20	Reliability evaluation of thermophysical properties from first-principles calculations. *Journal of Physics Condensed Matter*, **2014**, 26, 335401	1.8	8
19	Short-range order in face-centered cubic VCoNi alloys. *Physical Review Materials*, **2020**, 4,	3.2	8
18	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,	3.3	7
17	Element-resolved local lattice distortion in complex concentrated alloys: An observable signature of electronic effects. *Acta Materialia*, **2021**, 216, 117135	8.4	7
16	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	9.1	7
15	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. *Npj Computational Materials*, **2021**, 7,	10.9	6
14	Phonons in magnetically disordered materials: Magnetic versus phononic time scales. *Physical Review B*, **2020**, 101,	3.3	5
13	B2 ordering in body-centered-cubic AlNbTiV refractory high-entropy alloys. *Physical Review Materials*, **2021**, 5,	3.2	5
12	A fully automated approach to calculate the melting temperature of elemental crystals. *Computational Materials Science*, **2021**, 187, 110065	3.2	4
11	Shear band-driven precipitate dispersion for ultrastrong ductile medium-entropy alloys. *Nature Communications*, **2021**, 12, 4703	17.4	4
10	A new type of temperature driven reorientation transition in magnetic thin films. *European Physical Journal B*, **2006**, 53, 463-469	1.2	3
9	Effects of Cr/Ni ratio on physical properties of Cr-Mn-Fe-Co-Ni high-entropy alloys. *Acta Materialia*, **2022**, 227, 117693	8.4	2
8	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. *Npj Computational Materials*, **2022**, 8,	10.9	2
7	Hidden Effects of Negative Stacking Fault Energies in Complex Concentrated Alloys. *Physical Review Letters*, **2021**, 126, 255502	7.4	2
6	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,	3.2	2
5	Iron-rich High Entropy Alloys **2021**, 389-421		1
4	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	1	1

3	Effect of solid-solution strengthening on deformation mechanisms and strain hardening in medium-entropy V1-xCrxCoNi alloys. *Journal of Materials Science and Technology*, **2021**, 108, 270-270	9.1	0
2	Design of compositionally complex catalysts: Role of surface segregation. *Journal of Materials Research and Technology*, **2021**, 14, 1830-1836	5.5	0
1	Cu cap layer on Ni8/Cu(001): reorientation and TC-shift. *European Physical Journal B*, **2008**, 65, 499-504	1.2	