Blazej Grabowski

List of Publications by Year
in descending order

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104	7,976	76196	48187
papers	citations	40 h-index	88 g-index

106	106	106	7558
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
2	A map for phase-change materials. Nature Materials, 2008, 7, 972-977.	13.3	637
3	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
4	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
5	Ab initioup to the melting point: Anharmonicity and vacancies in aluminum. Physical Review B, 2009, 79, .	1.1	232
6	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
7	Ab initiostudy of the thermodynamic properties of nonmagnetic elementary fcc metals: Exchange-correlation-related error bars and chemical trends. Physical Review B, 2007, 76, .	1.1	218
8	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
9	Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition. Physical Review B, 2015, 92, .	1.1	187
10	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. Acta Materialia, 2017, 123, 90-101.	3.8	161
11	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157
12	Lattice Distortions in the FeCoNiCrMn High Entropy Alloy Studied by Theory and Experiment. Entropy, 2016, 18, 321.	1.1	151
13	Origin of shear induced Î² to Ï‰ transition in Tiâ€“Nb-based alloys. Acta Materialia, 2015, 92, 55-63.	3.8	129
14	Understanding Anharmonicity in fcc Materials: From its Origin toabÂinitioStrategies beyond the Quasiharmonic Approximation. Physical Review Letters, 2015, 114, 195901.	2.9	115
15	The role of metastable LPSO building block clusters in phase transformations of an Mg-Y-Zn alloy. Acta Materialia, 2016, 112, 171-183.	3.8	104
16	Phonon broadening in high entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	100
17	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
18	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93

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19	Breakdown of the Arrhenius Law in Describing Vacancy Formation Energies: The Importance of Local Anharmonicity Revealed byAb initioThermodynamics. Physical Review X, 2014, 4, .	2.8	92
20	A machine learning approach to model solute grain boundary segregation. Npj Computational Materials, 2018, 4, .	3.5	89
21	Improved method of calculatingab initiohigh-temperature thermodynamic properties with application to ZrC. Physical Review B, 2015, 91, .	1.1	86
22	â€œTreasure mapsâ€•for magnetic high-entropy-alloys from theory and experiment. Applied Physics Letters, 2015, 107, .	1.5	84
23	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
24	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
25	Computationally-driven engineering of sublattice ordering in a hexagonal AlHfScTiZr high entropy alloy. Scientific Reports, 2017, 7, 2209.	1.6	71
26	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
27	Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels. Jom, 2014, 66, 1399-1405.	0.9	64
28	Deformationâ€Induced Martensite: A New Paradigm for Exceptional Steels. Advanced Materials, 2016, 28, 7753-7757.	11.1	61
29	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
30	High-temperature phonon stabilization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-uranium from relativistic first-principles theory. Physical Review B, 2012, 85, .	1.1	59
31	From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titaniumâ€“transition metal alloys. Acta Materialia, 2016, 113, 311-319.	3.8	58
32	Formation energies of point defects at finite temperatures. Physica Status Solidi (B): Basic Research, 2011, 248, 1295-1308.	0.7	56
33	Thermodynamic modelling of crystalline unary phases. Physica Status Solidi (B): Basic Research, 2014, 251, 14-32.	0.7	55
34	Efficient approach to compute melting properties fully from ab initio with application to Cu. Physical Review B, 2017, 96, .	1.1	53
35	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
36	Temperature-driven phase transitions from first principles including all relevant excitations: The fcc-to-bcc transition in Ca. Physical Review B, 2011, 84, .	1.1	52

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37	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	3.5	52
38	Calculating free energies of point defects from ab initio. Computational Materials Science, 2018, 148, 249-259.	1.4	47
39	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45
40	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
41	Ab initio modelling of solute segregation energies to a general grain boundary. Acta Materialia, 2017, 132, 138-148.	3.8	42
42	Dislocation slip transmission through a coherent Î£3{111} copper twin boundary: Strain rate sensitivity, activation volume and strength distribution function. Acta Materialia, 2018, 161, 412-419.	3.8	41
43	Self-Healing Metals. Advances in Polymer Science, 2016, , 387-407.	0.4	40
44	Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128, .	1.1	40
45	Dissecting functional degradation in NiTi shape memory alloys containing amorphous regions via atomistic simulations. Acta Materialia, 2021, 202, 331-349.	3.8	39
46	Ab Initioâ€Based Prediction of Phase Diagrams: Application to Magnetic Shape Memory Alloys. Advanced Engineering Materials, 2012, 14, 547-561.	1.6	37
47	Basal slip in Laves phases: The synchroshear dislocation. Scripta Materialia, 2019, 166, 134-138.	2.6	37
48	First-principles study of the thermodynamic and elastic properties of eutectic Feâ€“Ti alloys. Acta Materialia, 2012, 60, 1594-1602.	3.8	36
49	Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires. Acta Materialia, 2016, 111, 321-334.	3.8	35
50	Atomistic migration mechanisms of atomically flat, stepped, and kinked grain boundaries. Physical Review B, 2016, 94, .	1.1	33
51	Zr diffusion in BCC refractory high entropy alloys: A case of â€˜non-sluggishâ€™ diffusion behavior. Acta Materialia, 2022, 233, 117970.	3.8	33
52	High-entropy hydrides for fast and reversible hydrogen storage at room temperature: Binding-energy engineering via first-principles calculations and experiments. Acta Materialia, 2022, 236, 118117.	3.8	30
53	Multiscale description of dislocation induced nano-hydrides. Acta Materialia, 2015, 89, 50-59.	3.8	29
54	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

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55	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. Physica Status Solidi (B): Basic Research, 2015, 252, 1907-1924.	0.7	27
56	Phenomenon of ultra-fast tracer diffusion of Co in HCP high entropy alloys. Acta Materialia, 2020, 196, 220-230.	3.8	27
57	Mechanisms and kinetics of the migration of grain boundaries containing extended defects. Physical Review B, 2015, 92, .	1.1	24
58	Multiscale modeling of hydrogen enhanced homogeneous dislocation nucleation. Acta Materialia, 2016, 107, 144-151.	3.8	24
59	Thermomechanical response of NiTi shape-memory nanoprecipitates in TiV alloys. Physical Review Materials, 2017, 1, .	0.9	23
60	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. European Physical Journal Plus, 2011, 126, 1.	1.2	22
61	Ab initio prediction of vacancy energetics in HCP Al-Hf-Sc-Ti-Zr high entropy alloys and the subsystems. Acta Materialia, 2022, 227, 117677.	3.8	22
62	Structural anomaly in the high-entropy alloy ZrNbTiTaHf. Intermetallics, 2016, 68, 11-15.	1.8	21
63	Impact of local electrostatic field rearrangement on field ionization. Journal Physics D: Applied Physics, 2018, 51, 105601.	1.3	20
64	Phonon Lifetimes throughout the Brillouin Zone at Elevated Temperatures from Experiment andAbÂInitio. Physical Review Letters, 2019, 123, 235501.	2.9	20
65	Atomistic deformation behavior of single and twin crystalline Cu nanopillars with preexisting dislocations. Acta Materialia, 2020, 197, 54-68.	3.8	20
66	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
67	Combined ab initio, experimental, and CALPHAD approach for an improved thermodynamic evaluation of the Mgâ€“Si system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2012, 37, 77-86.	0.7	19
68	Thermodynamic modeling of chromium: strong and weak magnetic coupling. Journal of Physics Condensed Matter, 2013, 25, 425401.	0.7	18
69	Random phase approximation up to the melting point: Impact of anharmonicity and nonlocal many-body effects on the thermodynamics of Au. Physical Review B, 2015, 91, .	1.1	18
70	A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065.	1.4	18
71	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. Acta Materialia, 2016, 102, 241-250.	3.8	17
72	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	3.5	17

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73	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
74	GBÂcode: A grain boundary generation code. Journal of Open Source Software, 2018, 3, 900.	2.0	17
75	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:m study aided by machine learning potentials. Physical Review B, 2022, 105, .	1.1	16
76	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
77	A QM/MM approach for low-symmetry defects in metals. Computational Materials Science, 2016, 118, 259-268.	1.4	14
78	Impact of asymmetric martensite and austenite nucleation and growth behavior on the phase stability and hysteresis of freestanding shape-memory nanoparticles. Physical Review Materials, 2018, 2, .	0.9	14
79	Migration mechanisms of a faceted grain boundary. Physical Review Materials, 2018, 2, .	0.9	14
80	Low-temperature features in the heat capacity of unary metals and intermetallics for the example of bulk aluminum and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Al</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:m mathvariant="normal">Sc</mml:mi></mml:math>. Physical Review B, 2017, 95, .	1.1	12
81	Ab initiobased method to study structural phase transitions in dynamically unstable crystals, with new insights on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>transformation in titanium. Physical Review B, 2019, 100, .	1.1	12
82	Molecular dynamics simulations of screw dislocation mobility in bcc Nb. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 085007.	0.8	11
83	Recent Advances in Understanding Diffusion in Multiprincipal Element Systems. Annual Review of Materials Research, 2022, 52, 383-409.	4.3	11
84	The role of molybdenum in suppressing cold dwell fatigue in titanium alloys. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2017, 473, 20170189.	1.0	10
85	Advanced data mining in field ion microscopy. Materials Characterization, 2018, 146, 307-318.	1.9	10
86	Fast anharmonic free energy method with an application to vacancies in ZrC. Physical Review B, 2019, 100, .	1.1	10
87	Finite temperature ab initio calculated thermodynamic properties of orthorhombic Cr3C2. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2016, 53, 72-77.	0.7	9
88	Ab initio simulations of the surface free energy of TiN(001). Physical Review B, 2021, 103, .	1.1	9
89	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
90	Li₅Sn, the Most Lithium-Rich Binary Stannide: A Combined Experimental and Computational Study. Journal of the American Chemical Society, 2022, 144, 7096-7110.	6.6	7

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91	Structural, Magnetic and Catalytic Properties of a New Vacancy Ordered Perovskite Type Barium Cobaltate BaCoO_{2.67}. Chemistry - A European Journal, 2021, 27, 9763-9767.	1.7	6
92	High Fidelity Reconstruction of Experimental Field Ion Microscopy Data by Atomic Relaxation Simulations. Microscopy and Microanalysis, 2017, 23, 642-643.	0.2	5
93	Design of a Vâ€“Tiâ€“Ni alloy with superelastic nano-precipitates. Acta Materialia, 2020, 196, 710-722.	3.8	5
94	A Combined Experimental and First-Principles Based Assessment of Finite-Temperature Thermodynamic Properties of Intermetallic Al3Sc. Materials, 2021, 14, 1837.	1.3	5
95	Atomistic simulations of the deformation behavior of an Nb nanowire embedded in a NiTi shape memory alloy. Acta Materialia, 2022, 228, 117764.	3.8	5
96	Structural and Magnetic Properties of BaFeO_{2.667} Synthesized by Oxidizing BaFeO_{2.5} Obtained via Nebulized Spray Pyrolysis. Inorganic Chemistry, 2021, 60, 10923-10933.	1.9	4
97	Thermally-activated dislocation mobility in bcc metals: An accelerated molecular dynamics study. Computational Materials Science, 2021, 200, 110804.	1.4	4
98	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors. Materials Research Society Symposia Proceedings, 2012, 1444, 67.	0.1	3
99	Determination of symmetry reduced structures using a soft phonon analysis for magnetic shape memory alloys (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064219.	0.7	2
100	Approximating the impact of nuclear quantum effects on thermodynamic properties of crystalline solids by temperature remapping. Physical Review B, 2022, 105, .	1.1	2
101	Crystal structure and phase stability of Co2N: A combined first-principles and experimental study. Journal of Alloys and Compounds, 2021, 854, 156341.	2.8	1
102	Comprehensive Understanding of H Adsorption on MoO₃ from Systematic Ab Initio Simulations. Journal of Physical Chemistry C, 0, , .	1.5	1
103	First principles determination of phase transitions in magnetic shape memory alloys. Acta Crystallographica Section A: Foundations and Advances, 2008, 64, C96-C96.	0.3	0
104	Joining dissimilar metal of Ti and CoCrMo using directed energy deposition. Journal of Materials Science and Technology, 2021, 111, 99-99.	5.6	0