Blazej Grabowski

List of Publications by Year
in descending order

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	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
2	Magnetic Moment Tensor Potentials for collinear spin-polarized materials reproduce different magnetic states of bcc Fe. Npj Computational Materials, 2022, 8, .	3.5	52
3	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
4	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
5	Zr diffusion in BCC refractory high entropy alloys: A case of â€˜non-sluggishâ€™ diffusion behavior. Acta Materialia, 2022, 233, 117970.	3.8	33
6	Recent Advances in Understanding Diffusion in Multiprincipal Element Systems. Annual Review of Materials Research, 2022, 52, 383-409.	4.3	11
7	Approximating the impact of nuclear quantum effects on thermodynamic properties of crystalline solids by temperature remapping. Physical Review B, 2022, 105, .	1.1	2
8	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
9	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
10	Dissecting functional degradation in NiTi shape memory alloys containing amorphous regions via atomistic simulations. Acta Materialia, 2021, 202, 331-349.	3.8	39
11	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
12	Chemically induced local lattice distortions versus structural phase transformations in compositionally complex alloys. Npj Computational Materials, 2021, 7, .	3.5	17
13	A fully automated approach to calculate the melting temperature of elemental crystals. Computational Materials Science, 2021, 187, 110065.	1.4	18
14	A Combined Experimental and First-Principles Based Assessment of Finite-Temperature Thermodynamic Properties of Intermetallic Al3Sc. Materials, 2021, 14, 1837.	1.3	5
15	Ab initio simulations of the surface free energy of TiN(001). Physical Review B, 2021, 103, .	1.1	9
16	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
17	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
18	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

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19	Molecular dynamics simulations of screw dislocation mobility in bcc Nb. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 085007.	0.8	11
20	Thermally-activated dislocation mobility in bcc metals: An accelerated molecular dynamics study. Computational Materials Science, 2021, 200, 110804.	1.4	4
21	Joining dissimilar metal of Ti and CoCrMo using directed energy deposition. Journal of Materials Science and Technology, 2021, 111, 99-99.	5.6	0
22	Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128, .	1.1	40
23	Atomistic deformation behavior of single and twin crystalline Cu nanopillars with preexisting dislocations. Acta Materialia, 2020, 197, 54-68.	3.8	20
24	Design of a Vâ€“Tiâ€“Ni alloy with superelastic nano-precipitates. Acta Materialia, 2020, 196, 710-722.	3.8	5
25	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
26	Phenomenon of ultra-fast tracer diffusion of Co in HCP high entropy alloys. Acta Materialia, 2020, 196, 220-230.	3.8	27
27	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
28	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
29	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
30	Fast anharmonic free energy method with an application to vacancies in ZrC. Physical Review B, 2019, 100, .	1.1	10
31	Ab initio vibrational free energies including anharmonicity for multicomponent alloys. Npj Computational Materials, 2019, 5, .	3.5	79
32	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
33	Basal slip in Laves phases: The synchroshear dislocation. Scripta Materialia, 2019, 166, 134-138.	2.6	37
34	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
35	Phonon Lifetimes throughout the Brillouin Zone at Elevated Temperatures from Experiment andAbÂInitio. Physical Review Letters, 2019, 123, 235501.	2.9	20
36	Impact of local electrostatic field rearrangement on field ionization. Journal Physics D: Applied Physics, 2018, 51, 105601.	1.3	20

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37	Calculating free energies of point defects from ab initio. Computational Materials Science, 2018, 148, 249-259.	1.4	47
38	Advanced data mining in field ion microscopy. Materials Characterization, 2018, 146, 307-318.	1.9	10
39	A machine learning approach to model solute grain boundary segregation. Npj Computational Materials, 2018, 4, .	3.5	89
40	Temperature dependence of the stacking-fault Gibbs energy for Al, Cu, and Ni. Physical Review B, 2018, 98, .	1.1	61
41	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
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	Temperature dependence of the Gibbs energy of vacancy formation of fcc Ni. Physical Review B, 2018, 97, .	1.1	45
44	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
45	Migration mechanisms of a faceted grain boundary. Physical Review Materials, 2018, 2, .	0.9	14
46	GBÂcode: A grain boundary generation code. Journal of Open Source Software, 2018, 3, 900.	2.0	17
47	Ab initio modelling of solute segregation energies to a general grain boundary. Acta Materialia, 2017, 132, 138-148.	3.8	42
48	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
49	High Fidelity Reconstruction of Experimental Field Ion Microscopy Data by Atomic Relaxation Simulations. Microscopy and Microanalysis, 2017, 23, 642-643.	0.2	5
50	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
51	Efficient approach to compute melting properties fully from ab initio with application to Cu. Physical Review B, 2017, 96, .	1.1	53
52	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
53	Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. Acta Materialia, 2017, 136, 262-270.	3.8	275
54	Computationally-driven engineering of sublattice ordering in a hexagonal AlHfScTiZr high entropy alloy. Scientific Reports, 2017, 7, 2209.	1.6	71

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55	Atomic scale processes of phase transformations in nanocrystalline NiTi shape-memory alloys. Acta Materialia, 2017, 123, 90-101.	3.8	161
56	Phonon broadening in high entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	100
57	Thermomechanical response of NiTi shape-memory nanoprecipitates in TiV alloys. Physical Review Materials, 2017, 1, .	0.9	23
58	Lattice Distortions in the FeCoNiCrMn High Entropy Alloy Studied by Theory and Experiment. Entropy, 2016, 18, 321.	1.1	151
59	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
60	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
61	A QM/MM approach for low-symmetry defects in metals. Computational Materials Science, 2016, 118, 259-268.	1.4	14
62	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
63	Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires. Acta Materialia, 2016, 111, 321-334.	3.8	35
64	Self-Healing Metals. Advances in Polymer Science, 2016, , 387-407.	0.4	40
65	Deformationâ€Induced Martensite: A New Paradigm for Exceptional Steels. Advanced Materials, 2016, 28, 7753-7757.	11.1	61
66	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
67	Atomistic migration mechanisms of atomically flat, stepped, and kinked grain boundaries. Physical Review B, 2016, 94, .	1.1	33
68	Multiscale modeling of hydrogen enhanced homogeneous dislocation nucleation. Acta Materialia, 2016, 107, 144-151.	3.8	24
69	Structural anomaly in the high-entropy alloy ZrNbTiTaHf. Intermetallics, 2016, 68, 11-15.	1.8	21
70	Partitioning of Cr and Si between cementite and ferrite derived from first-principles thermodynamics. Acta Materialia, 2016, 102, 241-250.	3.8	17
71	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
72	Improved method of calculatingab initiohigh-temperature thermodynamic properties with application to ZrC. Physical Review B, 2015, 91, .	1.1	86

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73	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
74	Mechanisms and kinetics of the migration of grain boundaries containing extended defects. Physical Review B, 2015, 92, .	1.1	24
75	â€œTreasure mapsâ€•for magnetic high-entropy-alloys from theory and experiment. Applied Physics Letters, 2015, 107, .	1.5	84
76	Understanding Anharmonicity in fcc Materials: From its Origin toabÂinitioStrategies beyond the Quasiharmonic Approximation. Physical Review Letters, 2015, 114, 195901.	2.9	115
77	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
78	Multiscale description of dislocation induced nano-hydrides. Acta Materialia, 2015, 89, 50-59.	3.8	29
79	Origin of shear induced Î² to Ï‰ transition in Tiâ€“Nb-based alloys. Acta Materialia, 2015, 92, 55-63.	3.8	129
80	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
81	Structural stability and thermodynamics of CrN magnetic phases fromab initiocalculations and experiment. Physical Review B, 2014, 90, .	1.1	95
82	First-principles calculations for point defects in solids. Reviews of Modern Physics, 2014, 86, 253-305.	16.4	1,967
83	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
84	Thermodynamic modelling of crystalline unary phases. Physica Status Solidi (B): Basic Research, 2014, 251, 14-32.	0.7	55
85	Temperature Dependent Magnon-Phonon Coupling in bcc Fe from Theory and Experiment. Physical Review Letters, 2014, 113, 165503.	2.9	93
86	Ab Initio Based Understanding of the Segregation and Diffusion Mechanisms of Hydrogen in Steels. Jom, 2014, 66, 1399-1405.	0.9	64
87	Thermodynamic modeling of chromium: strong and weak magnetic coupling. Journal of Physics Condensed Matter, 2013, 25, 425401.	0.7	18
88	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
89	Advancing density functional theory to finite temperatures: methods and applications in steel design. Journal of Physics Condensed Matter, 2012, 24, 053202.	0.7	75
90	Atomic forces at finite magnetic temperatures: Phonons in paramagnetic iron. Physical Review B, 2012, 85, .	1.1	157

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91	Ab Initio Study of Advanced Metallic Nuclear Fuels for Fast Breeder Reactors. Materials Research Society Symposia Proceedings, 2012, 1444, 67.	0.1	3
92	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
93	Ab Initioâ€Based Prediction of Phase Diagrams: Application to Magnetic Shape Memory Alloys. Advanced Engineering Materials, 2012, 14, 547-561.	1.6	37
94	First-principles study of the thermodynamic and elastic properties of eutectic Feâ€“Ti alloys. Acta Materialia, 2012, 60, 1594-1602.	3.8	36
95	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
96	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. European Physical Journal Plus, 2011, 126, 1.	1.2	22
97	Formation energies of point defects at finite temperatures. Physica Status Solidi (B): Basic Research, 2011, 248, 1295-1308.	0.7	56
98	Ab initioup to the melting point: Anharmonicity and vacancies in aluminum. Physical Review B, 2009, 79, .	1.1	232
99	A map for phase-change materials. Nature Materials, 2008, 7, 972-977.	13.3	637
100	Free energy of bcc iron: Integratedab initioderivation of vibrational, electronic, and magnetic contributions. Physical Review B, 2008, 78, .	1.1	188
101	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
102	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
103	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
104	Comprehensive Understanding of H Adsorption on MoO₃ from Systematic Ab Initio Simulations. Journal of Physical Chemistry C, 0, , .	1.5	1