Markus Eisenbach

List of Publications by Year
in descending order

70	1,097	430874 18	434195 31
papers	citations	h-index	g-index

76	76	76	1775
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMP application experiences: Porting to accelerated nodes. Parallel Computing, 2022, 109, 102856.	2.1	14
2	Computationally Accelerated Discovery of High Entropy Pyrochlore Oxides. Chemistry of Materials, 2022, 34, 1459-1472.	6.7	14
3	Ab initio approaches to high-entropy alloys: a comparison of CPA, SQS, and supercell methods. Journal of Materials Science, 2022, 57, 10677-10690.	3.7	6
4	Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators MnBi₂Te₄ and MnBi₄Te₇ by Defect Engineering and Chemical Doping. Advanced Functional Materials, 2021, 31, 2006516.	14.9	68
5	Monte Carlo simulation of order-disorder transition in refractory high entropy alloys: A data-driven approach. Computational Materials Science, 2021, 187, 110135.	3.0	40
6	Non-local corrections to the typical medium theory of Anderson localization. Annals of Physics, 2021, , 168454.	2.8	2
7	Application of the locally self-consistent embedding approach to the Anderson model with non-uniform random distributions. Annals of Physics, 2021, 435, 168480.	2.8	2
8	A scalable algorithm for the optimization of neural network architectures. Parallel Computing, 2021, 104-105, 102788.	2.1	1
9	Fast and stable deep-learning predictions of material properties for solid solution alloys**. Journal of Physics Condensed Matter, 2021, 33, 084005.	1.8	6
10	Hands-on with OWL: the Oakâ€“Ridge Wangâ€“Landau Monte Carlo software suite. Journal of Physics: Conference Series, 2021, 2122, 012001.	0.4	0
11	Robust data-driven approach for predicting the configurational energy of high entropy alloys. Materials and Design, 2020, 185, 108247.	7.0	40
12	Predicting the Phase Stability of Multicomponent High-Entropy Compounds. Chemistry of Materials, 2020, 32, 7507-7515.	6.7	37
13	Machine-learning-assisted insight into spin ice Dy2Ti2O7. Nature Communications, 2020, 11, 892.	12.8	58
14	Electron spin mediated distortion in metallic systems. Scripta Materialia, 2020, 185, 159-164.	5.2	3
15	Equilibrium solute segregation to matrix-Î¸â€² precipitate interfaces in Al-Cu alloys from first principles. Physical Review Materials, 2020, 4, .	2.4	4
16	Integrating Deep Learning in Domain Sciences at Exascale. Communications in Computer and Information Science, 2020, , 35-50.	0.5	3
17	Dislocation core structures and Peierls stresses of the high-entropy alloy NiCoFeCrMn and its subsystems. Materials and Design, 2019, 180, 107955.	7.0	26
18	Locally self-consistent embedding approach for disordered electronic systems. Physical Review B, 2019, 100, .	3.2	1

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19	First-principles study of order-disorder transitions in multicomponent solid-solution alloys. Journal of Physics Condensed Matter, 2019, 31, 273002.	1.8	7
20	Histogram-free multicanonical Monte Carlo sampling to calculate the density of states. Computer Physics Communications, 2019, 235, 297-304.	7.5	4
21	Error controlling of the combined Cluster-Expansion and Wangâ€“Landau Monte-Carlo method and its application to FeCo. Computer Physics Communications, 2019, 235, 95-101.	7.5	10
22	Hidden Mn magnetic-moment disorder and its influence on the physical properties of medium-entropy NiCoMn solid solution alloys. Physical Review Materials, 2019, 3, .	2.4	14
23	Fully-relativistic full-potential multiple scattering theory: A pathology-free scheme. Computer Physics Communications, 2018, 224, 265-272.	7.5	1
24	Transition from the twinning induced plasticity to the Î³-Îµ transformation induced plasticity in a high manganese steel. Acta Materialia, 2018, 161, 273-284.	7.9	17
25	Atomic Electron Tomography: Adding a New Dimension to See Single Atoms in Materials. Microscopy and Microanalysis, 2018, 24, 558-559.	0.4	0
26	Deciphering chemical order/disorder and material properties at the single-atom level. Nature, 2017, 542, 75-79.	27.8	243
27	Large-Scale Calculations for Material Sciences Using Accelerators to Improve Time- and Energy-to-Solution. Computing in Science and Engineering, 2017, 19, 83-85.	1.2	0
28	A new scaling approach for the mesoscale simulation of magnetic domain structures using Monte Carlo simulations. Journal of Magnetism and Magnetic Materials, 2017, 432, 42-48.	2.3	3
29	Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects. Scientific Reports, 2017, 7, 43482.	3.3	57
30	Acceleration of the Particle Swarm Optimization for Peierlsâ€“Nabarro modeling of dislocations in conventional and high-entropy alloys. Computer Physics Communications, 2017, 215, 7-12.	7.5	14
31	Collective dynamics in atomistic models with coupled translational and spin degrees of freedom. Physical Review B, 2017, 95, .	3.2	22
32	A Histogram-Free Multicanonical Monte Carlo Algorithm for the Basis Expansion of Density of States. , 2017, , .		0
33	GPU acceleration of the Locally Selfconsistent Multiple Scattering code for first principles calculation of the ground state and statistical physics of materials. Computer Physics Communications, 2017, 211, 2-7.	7.5	17
34	Atomic Electron Tomography: Probing 3D Structure and Material Properties at the Single-Atom Level. Microscopy and Microanalysis, 2017, 23, 1886-1887.	0.4	0
35	Combined molecular and spin dynamics simulation of bcc iron with lattice vacancies. Journal of Physics: Conference Series, 2017, 921, 012007.	0.4	4
36	Real-Space Multiple-Scattering Theory and Its Applications at Exascale. , 2017, , 449-460.		1

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37	A full-potential approach to the relativistic single-site Greenâ€™s function. Journal of Physics Condensed Matter, 2016, 28, 355501.	1.8	2
38	Density-functional Monte-Carlo simulation of CuZn order-disorder transition. Physical Review B, 2016, 93, .	3.2	26
39	Reinventing atomistic magnetic simulations with spin-orbit coupling. Physical Review B, 2016, 93, .	3.2	32
40	Magnetic Materials at finite Temperatures: thermodynamics and combined spin and molecular dynamics derived from first principles calculations. Journal of Physics: Conference Series, 2015, 640, 012019.	0.4	3
41	Exploring Replica-Exchange Wang-Landau sampling in higher-dimensional parameter space. Journal of Physics: Conference Series, 2015, 640, 012006.	0.4	9
42	CUDA Grid-Level Task Progression Algorithms. , 2015, , .		0
43	Accelerated application development: The ORNL Titan experience. Computers and Electrical Engineering, 2015, 46, 123-138.	4.8	26
44	Alignment of iron nanoparticles in a magnetic field due to shape anisotropy. Journal of Magnetism and Magnetic Materials, 2015, 394, 481-490.	2.3	7
45	Phonon-magnon interactions in body centered cubic iron: A combined molecular and spin dynamics study. Journal of Applied Physics, 2014, 115, 17D124.	2.5	19
46	Performance of Replica-exchange Wang-landau Sampling for the 2D Ising Model: A Brief Survey. Physics Procedia, 2014, 57, 43-47.	1.2	2
47	Combined molecular dynamics-spin dynamics simulations of bcc iron. Journal of Physics: Conference Series, 2014, 487, 012007.	0.4	5
48	Exact Enumeration of the Phase Space of an Ising Model of Ni$_{2}$MnGa. IEEE Transactions on Magnetics, 2013, 49, 3141-3143.	2.1	0
49	Toward Abstracting the Communication Intent in Applications to Improve Portability and Productivity. , 2013, , .		0
50	Effect of longitudinal degree of freedom of magnetic moment in body-centered-cubic iron. Journal of Applied Physics, 2013, 113, .	2.5	1
51	Effect of lattice vibrations on magnetic phase transition in bcc iron. Physical Review B, 2012, 86, .	3.2	46
52	Convergence for the Wang-Landau density of states. Physical Review E, 2011, 84, 065702.	2.1	17
53	First principles approach to the magneto caloric effect: Application toNi₂MnGa. Journal of Applied Physics, 2011, 109, 07A942.	2.5	11
54	A study of radiation damage effects on the magnetic structure of bulk Iron. Journal of Applied Physics, 2011, 109, 07E120.	2.5	2

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55	First principles calculation of finite temperature magnetism in Fe and Fe3C. Journal of Applied Physics, 2011, 109, 07E138.	2.5	24
56	Calculated electronic and magnetic structure of screw dislocations in alpha iron. Journal of Applied Physics, 2011, 109, 07E159.	2.5	8
57	Improved methods for calculating thermodynamic properties of magnetic systems using Wang-Landau density of states. Journal of Applied Physics, 2011, 109, 07E161.	2.5	2
58	Perturbation calculation of thermodynamic density of states. Physical Review E, 2011, 84, 061116.	2.1	1
59	A Theoretical Study of the Magnetic Structure of Bulk Iron with Radiation Defects. Materials Research Society Symposia Proceedings, 2011, 1363, 1.	0.1	0
60	Invar effect and noncollinear magnetism in FeCu alloys. Journal of Applied Physics, 2009, 105, .	2.5	6
61	A scalable method for ab initio computation of free energies in nanoscale systems. , 2009, , .		14
62	Noncollinear magnetism in Permalloy. Journal of Applied Physics, 2007, 101, 09G503.	2.5	0
63	On calculating the magnetic state of nanostructures. Progress in Materials Science, 2007, 52, 371-387.	32.8	18
64	Electronic and Magnetic Structure of ${m L}1_{0}$-FePt Nanoparticle Embedded in FePt Random Alloy. IEEE Transactions on Magnetics, 2007, 43, 3103-3105.	2.1	6
65	Epitaxial Stabilization of Ferromagnetism in the Nanophase of FeGe. Physical Review Letters, 2006, 96, 127201.	7.8	19
66	Intrinsic volume scaling of thermoinduced magnetization in antiferromagnetic nanoparticles. Physical Review B, 2005, 72, .	3.2	8
67	Magnetic structure of iron inclusions in copper. Journal of Applied Physics, 2004, 95, 6684-6686.	2.5	0
68	Magnetic anisotropy of monoatomic iron chains embedded in copper. Physical Review B, 2002, 65, .	3.2	35
69	Magnetic anisotropy of iron chains embedded in copper. Journal of Applied Physics, 2002, 91, 6878.	2.5	0
70	On the states of orientations along a magnetically inhomogeneous nanowire. Journal of Magnetism and Magnetic Materials, 2000, 208, 137-143.	2.3	5