

Bharat K Medasani

List of Publications by Year in descending order

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Version: 2024-02-01

22
papers

1,224
citations

567281

15
h-index

677142

22
g-index

22
all docs

22
docs citations

22
times ranked

2147
citing authors

#	ARTICLE	IF	CITATIONS
1	FireWorks: a dynamic workflow system designed for high-throughput applications. <i>Concurrency Computation Practice and Experience</i> , 2015, 27, 5037-5059.	2.2	373
2	Theoretical study of the surface energy, stress, and lattice contraction of silver nanoparticles. <i>Physical Review B</i> , 2007, 75, .	3.2	147
3	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators. <i>Computer Physics Communications</i> , 2018, 226, 165-179.	7.5	142
4	Predicting defect behavior in B2 intermetallics by merging ab initio modeling and machine learning. <i>Npj Computational Materials</i> , 2016, 2, .	8.7	90
5	Vacancy formation energies in metals: A comparison of MetaGGA with LDA and GGA exchange-correlation functionals. <i>Computational Materials Science</i> , 2015, 101, 96-107.	3.0	69
6	Computational study of the surface properties of aluminum nanoparticles. <i>Surface Science</i> , 2009, 603, 2042-2046.	1.9	58
7	Early stage structural development of prototypical zeolitic imidazolate framework (ZIF) in solution. <i>Nanoscale</i> , 2018, 10, 4291-4300.	5.6	56
8	<i>In Silico</i> Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. <i>Journal of Physical Chemistry C</i> , 2014, 118, 23790-23802.	3.1	40
9	SIMSOPT: A flexible framework for stellarator optimization. <i>Journal of Open Source Software</i> , 2021, 6, 3525.	4.6	39
10	Insight into Fluorocarbon Adsorption in Metal-Organic Frameworks via Experiments and Molecular Simulations. <i>Scientific Reports</i> , 2019, 9, 10289.	3.3	34
11	Ionic asymmetry and solvent excluded volume effects on spherical electric double layers: A density functional approach. <i>Journal of Chemical Physics</i> , 2014, 140, 204510.	3.0	33
12	Excluded volume and ion-ion correlation effects on the ionic atmosphere around B-DNA: Theory, simulations, and experiments. <i>Journal of Chemical Physics</i> , 2014, 141, 225103.	3.0	24
13	Vacancies and Vacancy-Mediated Self Diffusion in Cr_2O_3 : A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1817-1831.	3.1	24
14	First-Principles Investigation of Native Interstitial Diffusion in Cr_2O_3 . <i>Journal of Physical Chemistry C</i> , 2018, 122, 12984-12993.	3.1	19
15	PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds. <i>Computer Physics Communications</i> , 2015, 193, 118-123.	7.5	18
16	Defect and Dopant Mediated Thermoelectric Power Factor Tuning in Zn_4Sb_3 . <i>Advanced Electronic Materials</i> , 2020, 6, 1901284.	5.1	14
17	Temperature Dependence of Self-Diffusion in Cr_2O_3 from First Principles. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22139-22150.	3.1	12
18	Stellarator optimization for good magnetic surfaces at the same time as quasisymmetry. <i>Physics of Plasmas</i> , 2021, 28, .	1.9	12

#	ARTICLE	IF	CITATIONS
19	On the fast kinetics of B2 \leftrightarrow L21 ordering in Ni-Co-Mn-In metamagnetic shape memory alloys. Journal of Alloys and Compounds, 2019, 781, 479-489.	5.5	10
20	First \leftrightarrow Principles Characterization of Equilibrium Vacancy Concentration in Metamagnetic Shape Memory Alloys: An Example of Ni ₂ MnGa. Physica Status Solidi (B): Basic Research, 2018, 255, 1700523.	1.5	6
21	Surface properties of silver and aluminum nanoclusters. Proceedings of SPIE, 2008, , .	0.8	2
22	Stable Pt clusters anchored to monovacancies on graphene sheets. MRS Communications, 2017, 7, 891-895.	1.8	2