Bharat K Medasani

List of Publications by Year
in descending order

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		567281	677142
22	1,224	15	22
papers	citations	h-index	g-index

22	22	22	2147
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stellarator optimization for good magnetic surfaces at the same time as quasisymmetry. Physics of Plasmas, 2021, 28, .	1.9	12
2	SIMSOPT: A flexible framework for stellarator optimization. Journal of Open Source Software, 2021, 6, 3525.	4.6	39
3	Defect and Dopant Mediated Thermoelectric Power Factor Tuning in Î²â€Zn₄Sb₃. Advanced Electronic Materials, 2020, 6, 1901284.	5.1	14
4	Insight into Fluorocarbon Adsorption in Metal-Organic Frameworks via Experiments and Molecular Simulations. Scientific Reports, 2019, 9, 10289.	3.3	34
5	Temperature Dependence of Self-Diffusion in Cr₂O₃ from First Principles. Journal of Physical Chemistry C, 2019, 123, 22139-22150.	3.1	12
6	On the fast kinetics of B2â€“L21 ordering in Ni-Co-Mn-In metamagnetic shape memory alloys. Journal of Alloys and Compounds, 2019, 781, 479-489.	5.5	10
7	PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators. Computer Physics Communications, 2018, 226, 165-179.	7.5	142
8	Early stage structural development of prototypical zeolitic imidazolate framework (ZIF) in solution. Nanoscale, 2018, 10, 4291-4300.	5.6	56
9	Firstâ€Principles Characterization of Equilibrium Vacancy Concentration in Metamagnetic Shape Memory Alloys: An Example of Ni₂MnGa. Physica Status Solidi (B): Basic Research, 2018, 255, 1700523.	1.5	6
10	First-Principles Investigation of Native Interstitial Diffusion in Cr₂O₃. Journal of Physical Chemistry C, 2018, 122, 12984-12993.	3.1	19
11	Vacancies and Vacancy-Mediated Self Diffusion in Cr₂O₃: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 1817-1831.	3.1	24
12	Stable Pt clusters anchored to monovacancies on graphene sheets. MRS Communications, 2017, 7, 891-895.	1.8	2
13	Predicting defect behavior in B2 intermetallics by merging ab initio modeling and machine learning. Npj Computational Materials, 2016, 2, .	8.7	90
14	FireWorks: a dynamic workflow system designed for highâ€throughput applications. Concurrency Computation Practice and Experience, 2015, 27, 5037-5059.	2.2	373
15	Vacancy formation energies in metals: A comparison of MetaGGA with LDA and GGA exchangeâ€“correlation functionals. Computational Materials Science, 2015, 101, 96-107.	3.0	69
16	PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds. Computer Physics Communications, 2015, 193, 118-123.	7.5	18
17	Excluded volume and ion-ion correlation effects on the ionic atmosphere around B-DNA: Theory, simulations, and experiments. Journal of Chemical Physics, 2014, 141, 225103.	3.0	24
18	Ionic asymmetry and solvent excluded volume effects on spherical electric double layers: A density functional approach. Journal of Chemical Physics, 2014, 140, 204510.	3.0	33

#	Article	IF	Citations
19	In Silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. Journal of Physical Chemistry C, 2014, 118, 23790-23802.	3.1	40
20	Computational study of the surface properties of aluminum nanoparticles. Surface Science, 2009, 603, 2042-2046.	1.9	58
21	Surface properties of silver and aluminum nanoclusters. Proceedings of SPIE, 2008, , .	0.8	2
22	Theoretical study of the surface energy, stress, and lattice contraction of silver nanoparticles. Physical Review B, 2007, 75, .	3.2	147