Bingqing Cheng

List of Publications by Year
in descending order

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Version: 2024-02-01

29	1,472	394421 19	501196 28
papers	citations	h-index	g-index

29	29	29	1622
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	BenchML: an extensible pipelining framework for benchmarking representations of materials and molecules at scale. Machine Learning: Science and Technology, 2022, 3, 040501.	5.0	2
2	High-pressure phase behaviors of titanium dioxide revealed by a Î”-learning potential. Journal of Chemical Physics, 2022, 156, 074106.	3.0	2
3	Ranking the information content of distance measures. , 2022, 1, .		13
4	Quantum-mechanical exploration of the phase diagram of water. Nature Communications, 2021, 12, 588.	12.8	32
5	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	47.7	287
6	Phase behaviours of superionic water at planetary conditions. Nature Physics, 2021, 17, 1228-1232.	16.7	26
7	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	27.8	2
8	Liquid water contains the building blocks of diverse ice phases. Nature Communications, 2020, 11, 5757.	12.8	50
9	Mapping Materials and Molecules. Accounts of Chemical Research, 2020, 53, 1981-1991.	15.6	71
10	Computing the Heat Conductivity of Fluids from Density Fluctuations. Physical Review Letters, 2020, 125, 130602.	7.8	20
11	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	27.8	83
12	Predicting the phase diagram of titanium dioxide with random search and pattern recognition. Physical Chemistry Chemical Physics, 2020, 22, 12697-12705.	2.8	22
13	Classical nucleation theory predicts the shape of the nucleus in homogeneous solidification. Journal of Chemical Physics, 2020, 152, 044103.	3.0	7
14	Ab initio thermodynamics of liquid and solid water. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1110-1115.	7.1	201
15	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
16	Computing the absolute Gibbs free energy in atomistic simulations: Applications to defects in solids. Physical Review B, 2018, 97, .	3.2	53
17	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. Physical Chemistry Chemical Physics, 2018, 20, 28732-28740.	2.8	25
18	Hydrogen Diffusion and Trapping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Iron: The Role of Quantum and Anharmonic Fluctuations. Physical Review Letters, 2018, 120, 225901.	7.8	26

#	Article	IF	Citations
19	Communication: Computing the Tolman length for solid-liquid interfaces. Journal of Chemical Physics, 2018, 148, 231102.	3.0	12
20	Bridging the gap between atomistic and macroscopic models of homogeneous nucleation. Journal of Chemical Physics, 2017, 146, 034106.	3.0	19
21	The Gibbs free energy of homogeneous nucleation: From atomistic nuclei to the planar limit. Journal of Chemical Physics, 2017, 147, 104707.	3.0	10
22	Nuclear Quantum Effects in Water at the Triple Point: Using Theory as a Link Between Experiments. Journal of Physical Chemistry Letters, 2016, 7, 2210-2215.	4.6	57
23	Solid-liquid interfacial free energy out of equilibrium. Physical Review B, 2015, 92, .	3.2	40
24	A new dislocation-density-function dynamics scheme for computational crystal plasticity by explicit consideration of dislocation elastic interactions. International Journal of Plasticity, 2015, 67, 1-25.	8.8	38
25	Direct path integral estimators for isotope fractionation ratios. Journal of Chemical Physics, 2014, 141, 244112.	3.0	30
26	The sintering and densification behaviour of many copper nanoparticles: A molecular dynamics study. Computational Materials Science, 2013, 74, 1-11.	3.0	63
27	Crystal plasticity of Cu nanocrystals during collision. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 585, 326-334.	5.6	9
28	The crystal structures of sintered copper nanoparticles: A molecular dynamics study. International Journal of Plasticity, 2013, 47, 65-79.	8.8	40
29	Thermally induced solid-solid structural transition of copper nanoparticles through direct geometrical conversion. Journal of Chemical Physics, 2013, 138, 164314.	3.0	12