Bingqing Cheng

List of Publications by Year
in descending order

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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	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. Chemical Reviews, 2021, 121, 9816-9872.	47.7	287
2	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	7.5	220
3	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
4	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	27.8	83
5	Mapping Materials and Molecules. Accounts of Chemical Research, 2020, 53, 1981-1991.	15.6	71
6	The sintering and densification behaviour of many copper nanoparticles: A molecular dynamics study. Computational Materials Science, 2013, 74, 1-11.	3.0	63
7	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
8	Computing the absolute Gibbs free energy in atomistic simulations: Applications to defects in solids. Physical Review B, 2018, 97, .	3.2	53
9	Liquid water contains the building blocks of diverse ice phases. Nature Communications, 2020, 11, 5757.	12.8	50
10	The crystal structures of sintered copper nanoparticles: A molecular dynamics study. International Journal of Plasticity, 2013, 47, 65-79.	8.8	40
11	Solid-liquid interfacial free energy out of equilibrium. Physical Review B, 2015, 92, .	3.2	40
12	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
13	Quantum-mechanical exploration of the phase diagram of water. Nature Communications, 2021, 12, 588.	12.8	32
14	Direct path integral estimators for isotope fractionation ratios. Journal of Chemical Physics, 2014, 141, 244112.	3.0	30
15	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
16	Phase behaviours of superionic water at planetary conditions. Nature Physics, 2021, 17, 1228-1232.	16.7	26
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	Predicting the phase diagram of titanium dioxide with random search and pattern recognition. Physical Chemistry Chemical Physics, 2020, 22, 12697-12705.	2.8	22

#	Article	IF	Citations
19	Computing the Heat Conductivity of Fluids from Density Fluctuations. Physical Review Letters, 2020, 125, 130602.	7.8	20
20	Bridging the gap between atomistic and macroscopic models of homogeneous nucleation. Journal of Chemical Physics, 2017, 146, 034106.	3.0	19
21	Ranking the information content of distance measures. , 2022, 1, .		13
22	Thermally induced solid-solid structural transition of copper nanoparticles through direct geometrical conversion. Journal of Chemical Physics, 2013, 138, 164314.	3.0	12
23	Communication: Computing the Tolman length for solid-liquid interfaces. Journal of Chemical Physics, 2018, 148, 231102.	3.0	12
24	The Gibbs free energy of homogeneous nucleation: From atomistic nuclei to the planar limit. Journal of Chemical Physics, 2017, 147, 104707.	3.0	10
25	Crystal plasticity of Cu nanocrystals during collision. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 585, 326-334.	5.6	9
26	Classical nucleation theory predicts the shape of the nucleus in homogeneous solidification. Journal of Chemical Physics, 2020, 152, 044103.	3.0	7
27	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
28	High-pressure phase behaviors of titanium dioxide revealed by a Î”-learning potential. Journal of Chemical Physics, 2022, 156, 074106.	3.0	2
29	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	27.8	2