

Christopher J Knight

List of Publications by Year in descending order

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21
papers

856
citations

623734

14
h-index

677142

22
g-index

22
all docs

22
docs citations

22
times ranked

1113
citing authors

#	ARTICLE	IF	CITATIONS
1	On the accuracy of the MB-pol many-body potential for water: Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice. <i>Journal of Chemical Physics</i> , 2016, 145, 194504.	3.0	214
2	Hydrogen-Bond Topology and the IceVII/VIII and IceIh/XI Proton-Ordering Phase Transitions. <i>Physical Review Letters</i> , 2005, 94, 135701.	7.8	86
3	Molecular Origin of the Vibrational Structure of Ice I _h . <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2579-2583.	4.6	66
4	An analysis of hydrated proton diffusion in <i>ab initio</i> molecular dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 014104.	3.0	63
5	Many-Body Interactions in Ice. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1778-1784.	5.3	60
6	Hydrogen bond topology and the ice VII/VIII and IceIh/XI proton ordering phase transitions. <i>Physical Review E</i> , 2006, 73, 056113.	2.1	59
7	The Dissociated Amorphous Silica Surface: Model Development and Evaluation. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3456-3471.	5.3	45
8	Prediction of a Phase Transition to a Hydrogen Bond Ordered Form of Ice VI. <i>Journal of Physical Chemistry B</i> , 2005, 109, 21040-21046.	2.6	41
9	A reexamination of the ice III/IX hydrogen bond ordering phase transition. <i>Journal of Chemical Physics</i> , 2006, 125, 064506.	3.0	33
10	Vapor-liquid equilibrium of water with the MB-pol many-body potential. <i>Journal of Chemical Physics</i> , 2021, 154, 211103.	3.0	32
11	Hydrogen bond ordering in ice V and the transition to ice XIII. <i>Journal of Chemical Physics</i> , 2008, 129, 164513.	3.0	29
12	The role of transient resonances for ultra-fast imaging of single sucrose nanoclusters. <i>Nature Communications</i> , 2020, 11, 167.	12.8	27
13	Communication: Improved <i>ab initio</i> molecular dynamics by minimally biasing with experimental data. <i>Journal of Chemical Physics</i> , 2017, 146, 041102.	3.0	20
14	Anharmonic Rovibrational Partition Functions at High Temperatures: Tests of Reduced-Dimensional Models for Systems with up to Three Fluxional Modes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 6210-6228.	2.5	16
15	Atomistic three-dimensional coherent x-ray imaging of nonbiological systems. <i>Physical Review A</i> , 2016, 94, .	2.5	15
16	Large-scale atomistic calculations of clusters in intense x-ray pulses. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2017, 50, 104003.	1.5	14
17	Site Disorder in Ice VII Arising from Hydrogen Bond Fluctuations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12433-12438.	2.5	9
18	The behavior of methane-water mixtures under elevated pressures from simulations using many-body potentials. <i>Journal of Chemical Physics</i> , 2022, 156, .	3.0	7

#	ARTICLE	IF	CITATIONS
19	Rendezvous algorithms for large-scale modeling and simulation. Journal of Parallel and Distributed Computing, 2021, 147, 184-195.	4.1	3
20	Fluorescence intensity correlation imaging with high spatial resolution and elemental contrast using intense x-ray pulses. Structural Dynamics, 2021, 8, 044101.	2.3	3
21	Extended x-ray emission times of clusters in intense x-ray pulses. Physical Review A, 2020, 101, .	2.5	2