Christian J Burnham

List of Publications by Year in Descending Order

30 papers	1,942 citations	15 h-index	30 g-index
30 ext. papers	2,043 ext. citations	4 avg, IF	4.76 L-index

#	Paper	IF	Citations
30	Intra-Cage Structure, Vibrations and Tetrahedral-Site Hopping of H2 and D2 in Doubly-Occupied 51264 Cages in sII Clathrate Hydrates from Path-Integral and Classical Molecular Dynamics. *Applied Sciences (Switzerland)*, **2021**, 11, 54	2.6	1
29	Stability-Ranking of Crystalline Ice Polymorphs Using Density-Functional Theory. *Crystals*, **2020**, 10, 40	2.3	1
28	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from Schrödinger Equation Treatment. *Applied Sciences (Switzerland)*, **2020**, 10, 8504	2.6	1
27	Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study. *Physical Chemistry Chemical Physics*, **2019**, 21, 3339-3346	3.6	11
26	Crystal Structure Prediction via Basin-Hopping Global Optimization Employing Tiny Periodic Simulation Cells, with Application to Water-Ice. *Journal of Chemical Theory and Computation*, **2019**, 15, 3889-3900	6.4	9
25	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. *Molecular Physics*, **2019**, 117, 3241-3253	1.7	1
24	A New Relatively Simple Approach to Multipole Interactions in Either Spherical Harmonics or Cartesians, Suitable for Implementation into Ewald Sums. *International Journal of Molecular Sciences*, **2019**, 21,	6.3	2
23	Electro-nucleation of water nano-droplets in No Man's Land to fault-free ice I. *Physical Chemistry Chemical Physics*, **2018**, 20, 8042-8053	3.6	15
22	Electro-suppression of water nano-droplets' solidification in no man's land: Electromagnetic fields' entropic trapping of supercooled water. *Journal of Chemical Physics*, **2018**, 148, 044503	3.9	3
21	Study of hydrogen-molecule guests in type II clathrate hydrates using a force-matched potential model parameterised from ab initio molecular dynamics. *Journal of Chemical Physics*, **2018**, 148, 102323	3.9	16
20	Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4. *ACS Omega*, **2018**, 3, 15361-15369	3.9	14
19	Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study. *Journal of Chemical Physics*, **2018**, 149, 245102	3.9	17
18	Does Local Structure Bias How a Crystal Nucleus Evolves?. *Journal of Physical Chemistry Letters*, **2018**, 9, 6991-6998	6.4	12
17	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. *Journal of Physical Chemistry C*, **2017**, 121, 3690-3696	3.8	21
16	Ice-Amorphization of Supercooled Water Nanodroplets in No Man's Land. *ACS Earth and Space Chemistry*, **2017**, 1, 187-196	3.2	10
15	Electropumping of Water Through Human Aquaporin 4 by Circularly Polarized Electric Fields: Dramatic Enhancement and Control Revealed by Non-Equilibrium Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 4646-4651	6.4	8
14	Dynamics of hydrogen guests in ice XVII nanopores. *Physical Review Materials*, **2017**, 1,	3.2	6

13	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. *Physical Chemistry Chemical Physics*, **2016**, 19, 717-728	3.6	24
12	Free-Energy Calculations of the Intercage Hopping Barriers of Hydrogen Molecules in Clathrate Hydrates. *Journal of Physical Chemistry C*, **2016**, 120, 16561-16567	3.8	35
11	Communication: Librational dynamics in water, sI and sII clathrate hydrates, and ice Ih: Molecular-dynamics insights. *Journal of Chemical Physics*, **2016**, 144, 051101	3.9	10
10	Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	20
9	Study of clathrate hydrates via equilibrium molecular-dynamics simulation employing polarisable and non-polarisable, rigid and flexible water models. *Journal of Chemical Physics*, **2016**, 144, 164503	3.9	22
8	Molecular Dynamics Simulation of Ionic Liquids: The Effect of Electronic Polarizability. *Journal of Physical Chemistry B*, **2004**, 108, 11877-11881	3.4	367
7	On the importance of zero-point effects in molecular level classical simulations of water. *Journal of Molecular Liquids*, **2004**, 110, 177-192	6	9
6	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: a new method for force-matching. *Journal of Chemical Physics*, **2004**, 120, 10896-913	3.9	349
5	The formation of cyclic water complexes by sequential ring insertion: Experiment and theory. *Journal of Chemical Physics*, **2002**, 117, 1109-1122	3.9	124
4	Development of transferable interaction models for water. I. Prominent features of the water dimer potential energy surface. *Journal of Chemical Physics*, **2002**, 116, 1479-1492	3.9	116
3	Development of transferable interaction models for water. II. Accurate energetics of the first few water clusters from first principles. *Journal of Chemical Physics*, **2002**, 116, 1493-1499	3.9	342
2	Development of transferable interaction models for water. III. Reparametrization of an all-atom polarizable rigid model (TTM2-R) from first principles. *Journal of Chemical Physics*, **2002**, 116, 1500-1510	3.9	160
1	The parametrization of a Thole-type all-atom polarizable water model from first principles and its application to the study of water clusters (n=2-21) and the phonon spectrum of ice Ih. *Journal of Chemical Physics*, **1999**, 110, 4566-4581	3.9	216