

# Christian J Burnham

## List of Publications by Citations

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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	Molecular Dynamics Simulation of Ionic Liquids: The Effect of Electronic Polarizability. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 11877-11881	3.4	367
29	Effective force fields for condensed phase systems from ab initio molecular dynamics simulation: a new method for force-matching. <i>Journal of Chemical Physics</i> , <b>2004</b> , 120, 10896-913	3.9	349
28	Development of transferable interaction models for water. II. Accurate energetics of the first few water clusters from first principles. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 1493-1499	3.9	342
27	The parametrization of a Thole-type all-atom polarizable water model from first principles and its application to the study of water clusters (n=201) and the phonon spectrum of ice Ih. <i>Journal of Chemical Physics</i> , <b>1999</b> , 110, 4566-4581	3.9	216
26	Development of transferable interaction models for water. III. Reparametrization of an all-atom polarizable rigid model (TTM2B) from first principles. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 1500-1510	3.9	160
25	The formation of cyclic water complexes by sequential ring insertion: Experiment and theory. <i>Journal of Chemical Physics</i> , <b>2002</b> , 117, 1109-1122	3.9	124
24	Development of transferable interaction models for water. I. Prominent features of the water dimer potential energy surface. <i>Journal of Chemical Physics</i> , <b>2002</b> , 116, 1479-1492	3.9	116
23	Free-Energy Calculations of the Intercage Hopping Barriers of Hydrogen Molecules in Clathrate Hydrates. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 16561-16567	3.8	35
22	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 19, 717-728	3.6	24
21	Study of clathrate hydrates via equilibrium molecular-dynamics simulation employing polarisable and non-polarisable, rigid and flexible water models. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 164503	3.9	22
20	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 3690-3696	3.8	21
19	Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study. <i>International Journal of Molecular Sciences</i> , <b>2016</b> , 17,	6.3	20
18	Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study. <i>Journal of Chemical Physics</i> , <b>2018</b> , 149, 245102	3.9	17
17	Study of hydrogen-molecule guests in type II clathrate hydrates using a force-matched potential model parameterised from ab initio molecular dynamics. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 102323	3.9	16
16	Electro-nucleation of water nano-droplets in No Man's Land to fault-free ice I. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 8042-8053	3.6	15
15	Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4. <i>ACS Omega</i> , <b>2018</b> , 3, 15361-15369	3.9	14
14	Does Local Structure Bias How a Crystal Nucleus Evolves?. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6991-6998	6.4	12

13	Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 3339-3346	3.6	11
12	Ice-Amorphization of Supercooled Water Nanodroplets in No Man's Land. <i>ACS Earth and Space Chemistry</i> , <b>2017</b> , 1, 187-196	3.2	10
11	Communication: Librational dynamics in water, sI and sII clathrate hydrates, and ice Ih: Molecular-dynamics insights. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 051101	3.9	10
10	Crystal Structure Prediction via Basin-Hopping Global Optimization Employing Tiny Periodic Simulation Cells, with Application to Water-Ice. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 3889-3900	6.4	9
9	On the importance of zero-point effects in molecular level classical simulations of water. <i>Journal of Molecular Liquids</i> , <b>2004</b> , 110, 177-192	6	9
8	Electropumping of Water Through Human Aquaporin 4 by Circularly Polarized Electric Fields: Dramatic Enhancement and Control Revealed by Non-Equilibrium Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 4646-4651	6.4	8
7	Dynamics of hydrogen guests in ice XVII nanopores. <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	6
6	Electro-suppression of water nano-droplets' solidification in no man's land: Electromagnetic fields' entropic trapping of supercooled water. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 044503	3.9	3
5	A New Relatively Simple Approach to Multipole Interactions in Either Spherical Harmonics or Cartesians, Suitable for Implementation into Ewald Sums. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 21,	6.3	2
4	Stability-Ranking of Crystalline Ice Polymorphs Using Density-Functional Theory. <i>Crystals</i> , <b>2020</b> , 10, 40	2.3	1
3	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. <i>Molecular Physics</i> , <b>2019</b> , 117, 3241-3253	1.7	1
2	Intra-Cage Structure, Vibrations and Tetrahedral-Site Hopping of H <sub>2</sub> and D <sub>2</sub> in Doubly-Occupied 51264 Cages in sII Clathrate Hydrates from Path-Integral and Classical Molecular Dynamics. <i>Applied Sciences (Switzerland)</i> , <b>2021</b> , 11, 54	2.6	1
1	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from Schrödinger Equation Treatment. <i>Applied Sciences (Switzerland)</i> , <b>2020</b> , 10, 8504	2.6	1