Christopher J Fennell

List of Publications by Year
in descending order

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27 papers	1,836 citations	393982 19 h-index	500791 28 g-index
30 all docs	30 docs citations	30 times ranked	2329 citing authors

#	Article	IF	Citations
1	Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics. Journal of Chemical Physics, 2006, 124, 234104.	1.2	508
2	How Waterâ€™s Properties Are Encoded in Its Molecular Structure and Energies. Chemical Reviews, 2017, 117, 12385-12414.	23.0	284
3	Ion Pairing in Molecular Simulations of Aqueous Alkali Halide Solutions. Journal of Physical Chemistry B, 2009, 113, 6782-6791.	1.2	269
4	Charge Asymmetries in Hydration of Polar Solutes. Journal of Physical Chemistry B, 2008, 112, 2405-2414.	1.2	98
5	Modeling aqueous solvation with semi-explicit assembly. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3234-3239.	3.3	64
6	Simple Liquid Models with Corrected Dielectric Constants. Journal of Physical Chemistry B, 2012, 116, 6936-6944.	1.2	64
7	Structure of the Interfacial Region in Adsorbed Poly(vinyl acetate) on Silica. Macromolecules, 2016, 49, 298-307.	2.2	62
8	A Fixed-Charge Model for Alcohol Polarization in the Condensed Phase, and Its Role in Small Molecule Hydration. Journal of Physical Chemistry B, 2014, 118, 6438-6446.	1.2	54
9	Light Harvesting for Rapid and Selective Reactions: Click Chemistry with Strain-Loadable Alkenes. CheM, 2018, 4, 124-137.	5.8	47
10	Oil/Water Transfer Is Partly Driven by Molecular Shape, Not Just Size. Journal of the American Chemical Society, 2010, 132, 234-240.	6.6	45
11	Physical Modeling of Aqueous Solvation. Journal of Statistical Physics, 2011, 145, 209-226.	0.5	38
12	OOPSE: An object-oriented parallel simulation engine for molecular dynamics. Journal of Computational Chemistry, 2005, 26, 252-271.	1.5	37
13	Computational Free Energy Studies of a New Ice Polymorph Which Exhibits Greater Stability than Ice Ih. Journal of Chemical Theory and Computation, 2005, 1, 662-667.	2.3	34
14	Surface Bonding Is Stronger for Poly(methyl methacrylate) than for Poly(vinyl acetate). Macromolecules, 2016, 49, 4211-4219.	2.2	32
15	Field-SEA: A Model for Computing the Solvation Free Energies of Nonpolar, Polar, and Charged Solutes in Water. Journal of Physical Chemistry B, 2014, 118, 6431-6437.	1.2	30
16	Radical Perfluoroalkylation Enabled by a Catalytically Generated Halogen Bonding Complex and Visible Light Irradiation. Organic Letters, 2022, 24, 446-450.	2.4	27
17	On the structural and transport properties of the soft sticky dipole and related single-point water models. Journal of Chemical Physics, 2004, 120, 9175-9184.	1.2	21
18	Testing the semi-explicit assembly solvation model in the SAMPL3 community blind test. Journal of Computer-Aided Molecular Design, 2012, 26, 563-568.	1.3	20

#	Article	IF	Citations
19	Using Interpolation for Fast and Accurate Calculation of Ionâ€“Ion Interactions. Journal of Physical Chemistry B, 2014, 118, 8017-8025.	1.2	16
20	Two-dimensional molecular simulations using rose potentials. Journal of Molecular Liquids, 2017, 228, 11-18.	2.3	15
21	Small molecule solvation changes due to the presence of salt are governed by the cost of solvent cavity formation and dispersion. Journal of Chemical Physics, 2014, 141, 22D518.	1.2	12
22	Testing the semi-explicit assembly model of aqueous solvation in the SAMPL4 challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 259-264.	1.3	9
23	TRIFORCE: Tessellated Semianalytical Solvent Exposed Surface Areas and Derivatives. Journal of Chemical Theory and Computation, 2014, 10, 4121-4132.	2.3	8
24	Predicting water-to-cyclohexane partitioning of the SAMPL5 molecules using dielectric balancing of force fields. Journal of Computer-Aided Molecular Design, 2016, 30, 1059-1065.	1.3	8
25	Adapting the semi-explicit assembly solvation model for estimating water-cyclohexane partitioning with the SAMPL5 molecules. Journal of Computer-Aided Molecular Design, 2016, 30, 1067-1077.	1.3	3
26	Computational Signaling Protein Dynamics and Geometric Mass Relations in Biomolecular Diffusion. Journal of Physical Chemistry B, 2018, 122, 5599-5609.	1.2	1
27	Interactive Molecular Model Assembly with 3D Printing. Journal of Visualized Experiments, 2020, , .	0.2	1