Christopher J Fennell

List of Publications by Year
in descending order

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	Radical Perfluoroalkylation Enabled by a Catalytically Generated Halogen Bonding Complex and Visible Light Irradiation. Organic Letters, 2022, 24, 446-450.	2.4	27
2	Interactive Molecular Model Assembly with 3D Printing. Journal of Visualized Experiments, 2020, , .	0.2	1
3	Computational Signaling Protein Dynamics and Geometric Mass Relations in Biomolecular Diffusion. Journal of Physical Chemistry B, 2018, 122, 5599-5609.	1.2	1
4	Light Harvesting for Rapid and Selective Reactions: Click Chemistry with Strain-Loadable Alkenes. CheM, 2018, 4, 124-137.	5.8	47
5	How Waterâ€™s Properties Are Encoded in Its Molecular Structure and Energies. Chemical Reviews, 2017, 117, 12385-12414.	23.0	284
6	Two-dimensional molecular simulations using rose potentials. Journal of Molecular Liquids, 2017, 228, 11-18.	2.3	15
7	Surface Bonding Is Stronger for Poly(methyl methacrylate) than for Poly(vinyl acetate). Macromolecules, 2016, 49, 4211-4219.	2.2	32
8	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
9	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
10	Structure of the Interfacial Region in Adsorbed Poly(vinyl acetate) on Silica. Macromolecules, 2016, 49, 298-307.	2.2	62
11	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
12	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
13	Using Interpolation for Fast and Accurate Calculation of Ionâ€“Ion Interactions. Journal of Physical Chemistry B, 2014, 118, 8017-8025.	1.2	16
14	TRIFORCE: Tessellated Semianalytical Solvent Exposed Surface Areas and Derivatives. Journal of Chemical Theory and Computation, 2014, 10, 4121-4132.	2.3	8
15	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
16	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
17	Simple Liquid Models with Corrected Dielectric Constants. Journal of Physical Chemistry B, 2012, 116, 6936-6944.	1.2	64
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	Physical Modeling of Aqueous Solvation. Journal of Statistical Physics, 2011, 145, 209-226.	0.5	38
20	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
21	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
22	Ion Pairing in Molecular Simulations of Aqueous Alkali Halide Solutions. Journal of Physical Chemistry B, 2009, 113, 6782-6791.	1.2	269
23	Charge Asymmetries in Hydration of Polar Solutes. Journal of Physical Chemistry B, 2008, 112, 2405-2414.	1.2	98
24	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
25	OOPSE: An object-oriented parallel simulation engine for molecular dynamics. Journal of Computational Chemistry, 2005, 26, 252-271.	1.5	37
26	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
27	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