Frank C Pickard Iv

List of Publications by Year in Descending Order

31 papers	969 citations	18 h-index	31 g-index
32 ext. papers	1,076 ext. citations	5.5 avg, IF	3.99 L-index

#	Paper	IF	Citations
31	Kinetic Modeling of API Oxidation: (1) The AIBN/HO/CHOH Radical "Soup". *Molecular Pharmaceutics*, **2021**, 18, 3037-3049	5.6	5
30	Five Degrees of Separation: Characterization and Temperature Stability Profiles for the Polymorphs of PD-0118057 (Molecule XXIII). *Crystal Growth and Design*, **2021**, 21, 4435-4444	3.5	1
29	Interactions of Water and Alkanes: Modifying Additive Force Fields to Account for Polarization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 3854-3867	6.4	19
28	Structural Modulation of Human Amylin Protofilaments by Naturally Occurring Mutations. *Journal of Physical Chemistry B*, **2018**, 122, 5657-5665	3.4	10
27	Comparison of Additive and Polarizable Models with Explicit Treatment of Long-Range Lennard-Jones Interactions Using Alkane Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 948-958	6.4	31
26	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. *Molecules*, **2018**, 23,	4.8	23
25	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 679-695	6.4	14
24	Absolute binding free energies for octa-acids and guests in SAMPL5 : Evaluating binding free energies for octa-acid and guest complexes in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 107-118	4.2	15
23	Machine Learning Force Field Parameters from Ab Initio Data. *Journal of Chemical Theory and Computation*, **2017**, 13, 4492-4503	6.4	73
22	Mapping the Drude polarizable force field onto a multipole and induced dipole model. *Journal of Chemical Physics*, **2017**, 147, 161702	3.9	32
21	Absolute binding free energy calculations of CBClip host-guest systems in the SAMPL5 blind challenge. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 71-85	4.2	9
20	An efficient protocol for obtaining accurate hydration free energies using quantum chemistry and reweighting from molecular dynamics simulations. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 4988-4997	3.4	14
19	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 989-1006	4.2	20
18	Molecular Multipole Potential Energy Functions for Water. *Journal of Physical Chemistry B*, **2016**, 120, 1833-42	3.4	9
17	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. *Journal of Chemical Theory and Computation*, **2016**, 12, 332-44	6.4	36
16	An empirical extrapolation scheme for efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2016**, 145, 164101	3.9	24
15	Isotropic periodic sum for multipole interactions and a vector relation for calculation of the Cartesian multipole tensor. *Journal of Chemical Physics*, **2016**, 145, 164110	3.9	5

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14	Blind prediction of distribution in the SAMPL5 challenge with QM based protomer and pK corrections. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 1087-1100	4.2	24
13	Numerical study on the partitioning of the molecular polarizability into fluctuating charge and induced atomic dipole contributions. *Journal of Physical Chemistry A*, **2015**, 119, 5865-82	2.8	36
12	Efficient treatment of induced dipoles. *Journal of Chemical Physics*, **2015**, 143, 074115	3.9	34
11	Predicting hydration free energies with a hybrid QM/MM approach: an evaluation of implicit and explicit solvation models in SAMPL4. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 245-57	4.2	53
10	Web-based computational chemistry education with CHARMMing II: Coarse-grained protein folding. *PLoS Computational Biology*, **2014**, 10, e1003738	5	5
9	An efficient algorithm for multipole energies and derivatives based on spherical harmonics and extensions to particle mesh Ewald. *Journal of Chemical Physics*, **2014**, 140, 184101	3.9	41
8	Comparing normal modes across different models and scales: Hessian reduction versus coarse-graining. *Journal of Computational Chemistry*, **2012**, 33, 2250-75	3.5	12
7	Characterization of the HSiN_HNSi system in its electronic ground state. *Journal of Chemical Physics* , **2009**, 130, 104301	3.9	10
6	Capture of hydroxymethylene and its fast disappearance through tunnelling. *Nature*, **2008**, 453, 906-9	50.4	233
5	Efficient and accurate characterization of the Bergman cyclization for several enediynes including an expanded substructure of esperamicin A1. *Journal of Physical Chemistry B*, **2008**, 112, 16917-34	3.4	14
4	Ortho effect in the Bergman cyclization: electronic and steric effects in hydrogen abstraction by 1-substituted naphthalene 5,8-diradicals. *Journal of Physical Chemistry A*, **2006**, 110, 2517-26	2.8	43
3	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. *International Journal of Quantum Chemistry*, **2006**, 106, 3122-3128	2.1	26
2	Comparison of model chemistry and density functional theory thermochemical predictions with experiment for formation of ionic clusters of the ammonium cation complexed with water and ammonia; atmospheric implications. *Journal of Physical Chemistry A*, **2005**, 109, 4905-10	2.8	46
1	Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. *Journal of Chemical Physics*, **2005**, 122, 024302	3.9	50