Edward Harder

List of Publications by Year
in descending order

25 papers	6,933 citations	318942 23 h-index	651938 25 g-index
25 all docs	25 docs citations	25 times ranked	11246 citing authors

#	Article	IF	Citations
1	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. Journal of Chemical Information and Modeling, 2019, 59, 3955-3967.	2.5	23
2	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45
3	High Energy Density in Azobenzene-based Materials for Photo-Thermal Batteries via Controlled Polymer Architecture and Polymer-Solvent Interactions. Scientific Reports, 2017, 7, 17773.	1.6	31
4	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	1.6	108
5	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	2.3	2,349
6	How To Deal with Multiple Binding Poses in Alchemical Relative Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2670-2679.	2.3	54
7	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	1.2	159
8	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	1.0	1,426
9	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 2553-2558.	2.3	239
10	Computer simulations of water flux and salt permeability of the reverse osmosis FT-30 aromatic polyamide membrane. Journal of Membrane Science, 2011, 384, 1-9.	4.1	87
11	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
12	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	1.2	139
13	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	6.6	98
14	Formalisms for the Explicit Inclusion of Electronic Polarizability in Molecular Modeling and Dynamics Studies. Challenges and Advances in Computational Chemistry and Physics, 2009, , 219-257.	0.6	8
15	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	1.2	88
16	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122
17	Theoretical Study of Aqueous Solvation of K⁺ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	2.3	87
18	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	2.3	142

#	Article	IF	Citations
19	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	1.2	548
20	Polarizable molecules in the vibrational spectroscopy of water. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 11611-11616.	3.3	77
21	Structure and Dynamics of the Solvation of Bovine Pancreatic Trypsin Inhibitor in Explicit Water:â€‰ A Comparative Study of the Effects of Solvent and Protein Polarizability. Journal of Physical Chemistry B, 2005, 109, 16529-16538.	1.2	55
22	Efficient Simulation Method for Polarizable Protein Force Fields:â€‰ Application to the Simulation of BPTI in Liquid Water. Journal of Chemical Theory and Computation, 2005, 1, 169-180.	2.3	68
23	Hydrogen-Bond Dynamics in the Airâ^'Water Interface. Journal of Physical Chemistry B, 2005, 109, 2949-2955.	1.2	121
24	On the Calculation of Diffusion Coefficients in Confined Fluids and Interfaces with an Application to the Liquidâ^'Vapor Interface of Water. Journal of Physical Chemistry B, 2004, 108, 6595-6602.	1.2	337
25	Efficient multiple time step method for use with Ewald and particle mesh Ewald for large biomolecular systems. Journal of Chemical Physics, 2001, 115, 2348-2358.	1.2	121