Edward D Harder

List of Publications by Year
in descending order

17 papers	6,259 citations	516710 16 h-index	888059 17 g-index
17 all docs	17 docs citations	17 times ranked	9400 citing authors

#	Article	IF	Citations
1	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	5.3	2,349
2	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	2.0	1,426
3	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1863-1874.	5.3	698
4	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. Journal of Chemical Theory and Computation, 2021, 17, 4291-4300.	5.3	582
5	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.	5.3	239
6	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
7	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	2.6	139
8	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	2.6	122
9	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
10	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	13.7	98
11	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	3.0	88
12	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.	5.3	54
13	Enhancing Water Sampling in Free Energy Calculations with Grand Canonical Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 6061-6076.	5.3	53
14	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	5.4	45
15	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. Journal of Chemical Information and Modeling, 2019, 59, 3955-3967.	5.4	23
16	Transferable Neural Network Potential Energy Surfaces for Closed-Shell Organic Molecules: Extension to Ions. Journal of Chemical Theory and Computation, 2022, 18, 2354-2366.	5.3	16
17	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. Journal of Chemical Theory and Computation, 2020, 16, 6926-6937.	5.3	8