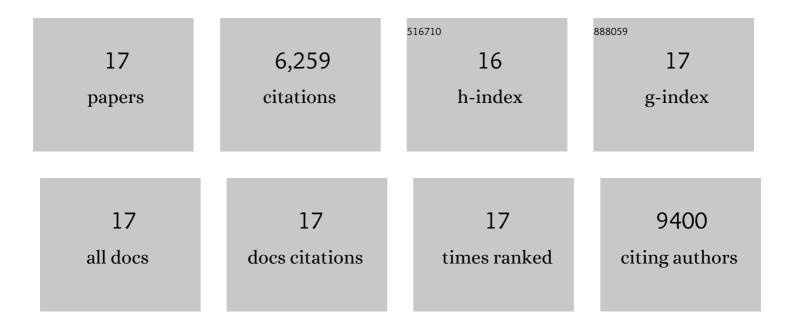
Edward D Harder

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/2018779/publications.pdf Version: 2024-02-01



#	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 Protein–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