

Edward D Harder

List of Publications by Year in descending order

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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	Transferable Neural Network Potential Energy Surfaces for Closed-Shell Organic Molecules: Extension to Ions. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2354-2366.	5.3	16
2	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4291-4300.	5.3	582
3	Enhancing Water Sampling in Free Energy Calculations with Grand Canonical Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6061-6076.	5.3	53
4	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6926-6937.	5.3	8
5	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3955-3967.	5.4	23
6	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1863-1874.	5.3	698
7	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 993-1004.	5.4	45
8	Advancing Drug Discovery through Enhanced Free Energy Calculations. <i>Accounts of Chemical Research</i> , 2017, 50, 1625-1632.	15.6	211
9	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. <i>ACS Omega</i> , 2016, 1, 293-304.	3.5	108
10	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 281-296.	5.3	2,349
11	How To Deal with Multiple Binding Poses in Alchemical Relative Protein-Ligand Binding Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2670-2679.	5.3	54
12	Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2110-2142.	2.0	1,426
13	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2553-2558.	5.3	239
14	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10177-10182.	2.6	139
15	Many-Body Polarization Effects and the Membrane Dipole Potential. <i>Journal of the American Chemical Society</i> , 2009, 131, 2760-2761.	13.7	98
16	On the origin of the electrostatic potential difference at a liquid-vacuum interface. <i>Journal of Chemical Physics</i> , 2008, 129, 234706.	3.0	88
17	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3509-3521.	2.6	122