Chuanjie Wu

List of Publications by Year
in descending order

20 papers	6,359 citations	516710 16 h-index	794594 19 g-index
20 all docs	20 docs citations	20 times ranked	8429 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	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
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	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	5.3	524
6	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3143-3161.	5.3	385
7	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	5.3	178
8	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	5.3	109
9	Molecular dynamics simulation guiding the improvement of EVA-type pour point depressant. Fuel, 2005, 84, 2039-2047.	6.4	88
10	Study on performance mechanism of pour point depressants with differential scanning calorimeter and X-ray diffraction methodsâ‹†. Fuel, 2003, 82, 1419-1426.	6.4	86
11	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	3.3	69
12	DFT and MM calculation: the performance mechanism of pour point depressants study. Fuel, 2004, 83, 315-326.	6.4	60
13	Reintroducing Electrostatics into Macromolecular Crystallographic Refinement: Application to Neutron Crystallography and DNA Hydration. Structure, 2011, 19, 523-533.	3.3	36
14	Molecular Dynamics of Î²-Hairpin Models of Epigenetic Recognition Motifs. Journal of the American Chemical Society, 2012, 134, 15970-15978.	13.7	29
15	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. Journal of Chemical Information and Modeling, 2019, 59, 3955-3967.	5.4	23
16	Artificial neural network model to predict cold filter plugging point of blended diesel fuels. Fuel Processing Technology, 2006, 87, 585-590.	7.2	18
17	Prediction of Henry's law constants of small gas molecules in liquid ethylene oxide and ethanol using force field methods. Fluid Phase Equilibria, 2005, 236, 66-77.	2.5	14
18	Prediction of the heat of mixing for binary fluids using molecular dynamics simulation. Fluid Phase Equilibria, 2005, 236, 78-85.	2.5	10

#	Article	IF	Citations
19	Mutual solubilities study for binary mixtures of dipropylene glycol dimethyl ether and water via molecular dynamics simulation and AMOEBA polarizable force field. Fluid Phase Equilibria, 2011, 310, 32-38.	2.5	8
20	An ab initio study of the alpha-fluorination effects on phosphatase inhibitors. Computational and Theoretical Chemistry, 2005, 726, 1-9.	1.5	0