Chuanjie Wu

List of Publications by Year
in descending order

20	6,359	516710	794594
papers	citations	16	19
		h-index	g-index

20	20	20	8429
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. Journal of Chemical Theory and Computation, 2021, 17, 4291-4300.	5.3	582
2	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. Journal of Chemical Information and Modeling, 2019, 59, 3955-3967.	5.4	23
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	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	5.3	178
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.	5.3	2,349
6	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	5.3	524
7	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	5.3	109
8	Molecular Dynamics of Î²-Hairpin Models of Epigenetic Recognition Motifs. Journal of the American Chemical Society, 2012, 134, 15970-15978.	13.7	29
9	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3143-3161.	5.3	385
10	Reintroducing Electrostatics into Macromolecular Crystallographic Refinement: Application to Neutron Crystallography and DNA Hydration. Structure, 2011, 19, 523-533.	3.3	36
11	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
12	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	3.3	69
13	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
14	Artificial neural network model to predict cold filter plugging point of blended diesel fuels. Fuel Processing Technology, 2006, 87, 585-590.	7.2	18
15	Molecular dynamics simulation guiding the improvement of EVA-type pour point depressant. Fuel, 2005, 84, 2039-2047.	6.4	88
16	An ab initio study of the alpha-fluorination effects on phosphatase inhibitors. Computational and Theoretical Chemistry, 2005, 726, 1-9.	1.5	0
17	Prediction of the heat of mixing for binary fluids using molecular dynamics simulation. Fluid Phase Equilibria, 2005, 236, 78-85.	2.5	10
18	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

#	Article	IF	Citations
19	DFT and MM calculation: the performance mechanism of pour point depressants study. Fuel, 2004, 83, 315-326.	6.4	60
20	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