

Wolfgang Damm

List of Publications by Year in descending order

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24
papers

8,979
citations

448610

19
h-index

759306

22
g-index

25
all docs

25
docs citations

25
times ranked

13159
citing authors

#	ARTICLE	IF	CITATIONS
1	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4291-4300.	2.3	582
2	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.	2.3	8
3	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1863-1874.	2.3	698
4	High Energy Density in Azobenzene-based Materials for Photo-Thermal Batteries via Controlled Polymer Architecture and Polymer-Solvent Interactions. <i>Scientific Reports</i> , 2017, 7, 17773.	1.6	31
5	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.	2.3	2,349
6	Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. <i>Journal of the American Chemical Society</i> , 2015, 137, 2695-2703.	6.6	931
7	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.	2.3	239
8	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1509-1519.	2.3	1,360
9	Explicit-Solvent Molecular Dynamics Simulations of the Polysaccharide Schizophyllan in Water. <i>Biophysical Journal</i> , 2007, 93, 442-455.	0.2	61
10	Integrated Modeling Program, Applied Chemical Theory (IMPACT). <i>Journal of Computational Chemistry</i> , 2005, 26, 1752-1780.	1.5	1,194
11	A Polarizable Force Field and Continuum Solvation Methodology for Modeling of Protein-Ligand Interactions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 694-715.	2.3	100
12	Explicit-Solvent Molecular Dynamics Simulations of the β (1 \rightarrow 3)- and β (1 \rightarrow 6)-Linked Disaccharides β -Laminarabiose and β -Gentiobiose in Water. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5815-5826.	1.2	32
13	Polarizable force fields. <i>Current Opinion in Structural Biology</i> , 2001, 11, 236-242.	2.6	474
14	Reversible peptide folding: Dependence on molecular force field used. <i>Journal of Computational Chemistry</i> , 2000, 21, 774-787.	1.5	19
15	Mechanistic Studies in the Radical Induced DNA Strand Cleavage-Formation and Reactivity of the Radical Cation Intermediate. <i>Tetrahedron</i> , 2000, 56, 4117-4128.	1.0	27
16	OPLS all-atom force field for carbohydrates. <i>Journal of Computational Chemistry</i> , 1997, 18, 1955-1970.	1.5	619
17	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		2
18	OPLS all-atom force field for carbohydrates. , 1997, 18, 1955.		26

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19	The Curtin-Hammett principle: Stereoselective radical additions to alkenes. <i>Tetrahedron Letters</i> , 1996, 37, 351-354.	0.7	44
20	Stereoselective reactions of α -imide substituted radicals. <i>Tetrahedron</i> , 1994, 50, 7029-7048.	1.0	19
21	Transition states for the hydrogen atom abstraction reaction by α -oxygen substituted radicals: Felkin-Anh Rule in Radical Chemistry. <i>Tetrahedron Letters</i> , 1993, 34, 431-434.	0.7	29
22	The Felkin-Anh Rule in Radical Chemistry: 1,2-Stereinduction in Radical Addition to Alkenes. <i>Synlett</i> , 1992, 1992, 441-443.	1.0	24
23	1,2-Stereinduction in acyclic radicals: allylic strain effects. <i>Tetrahedron Letters</i> , 1992, 33, 1863-1866.	0.7	62
24	Cram's rule for radical reactions. <i>Tetrahedron Letters</i> , 1991, 32, 6097-6100.	0.7	49