Ryan S Defever

List of Publications by Year
in descending order

16 papers	409 citations	759233 12 h-index	996975 15 g-index
16 all docs	16 docs citations	16 times ranked	578 citing authors

#	Article	IF	Citations
1	Suppression of sub-surface freezing in free-standing thin films of a coarse-grained model of water. Physical Chemistry Chemical Physics, 2014, 16, 25916-25927.	2.8	65
2	A generalized deep learning approach for local structure identification in molecular simulations. Chemical Science, 2019, 10, 7503-7515.	7.4	55
3	Mental Rolodexing: Senior Chemistry Majorsâ€™ Understanding of Chemical and Physical Properties. Journal of Chemical Education, 2015, 92, 415-426.	2.3	45
4	PAMAM Dendrimers and Graphene: Materials for Removing Aromatic Contaminants from Water. Environmental Science & Technology, 2015, 49, 4490-4497.	10.0	40
5	Free Energies of Catalytic Species Adsorbed to Pt(111) Surfaces under Liquid Solvent Calculated Using Classical and Quantum Approaches. Journal of Chemical Information and Modeling, 2019, 59, 2190-2198.	5.4	37
6	Nucleation mechanism of clathrate hydrates of water-soluble guest molecules. Journal of Chemical Physics, 2017, 147, 204503.	3.0	32
7	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 4400-4414.	5.4	29
8	Contour forward flux sampling: Sampling rare events along multiple collective variables. Journal of Chemical Physics, 2019, 150, 024103.	3.0	20
9	Comparison of fixed charge and polarizable models for predicting the structural, thermodynamic, and transport properties of molten alkali chlorides. Journal of Chemical Physics, 2020, 153, 214502.	3.0	19
10	Surface chemistry effects on heterogeneous clathrate hydrate nucleation: A molecular dynamics study. Journal of Chemical Thermodynamics, 2018, 117, 205-213.	2.0	17
11	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	3.6	16
12	Melting points of alkali chlorides evaluated for a polarizable and non-polarizable model. Journal of Chemical Physics, 2020, 153, 011101.	3.0	15
13	Association of small aromatic molecules with PAMAM dendrimers. Physical Chemistry Chemical Physics, 2015, 17, 29548-29557.	2.8	9
14	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. Journal of Computational Chemistry, 2021, 42, 1321-1331.	3.3	4
15	Building A Scalable Forward Flux Sampling Framework using Big Data and HPC. , 2019, , .		3
16	Computing the Liquidus of Binary Monatomic Salt Mixtures with Direct Simulation and Alchemical Free Energy Methods. Journal of Physical Chemistry A, 2021, 125, 8498-8513.	2.5	3