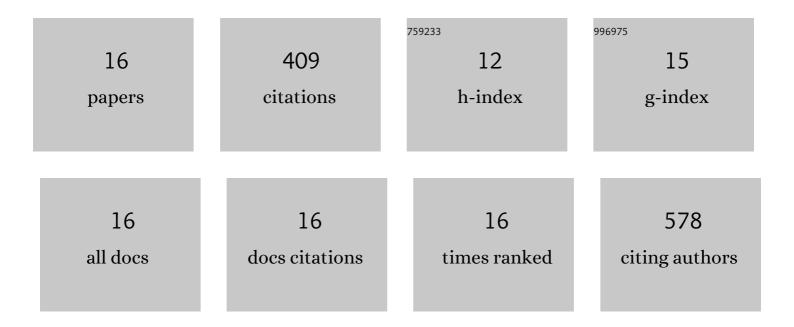
Ryan S Defever

List of Publications by Year in descending order

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RVAN S DEEEVED

#	Article	IF	CITATIONS
1	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	3.6	16
2	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. Journal of Computational Chemistry, 2021, 42, 1321-1331.	3.3	4
3	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 4400-4414.	5.4	29
4	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
5	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
6	Melting points of alkali chlorides evaluated for a polarizable and non-polarizable model. Journal of Chemical Physics, 2020, 153, 011101.	3.0	15
7	Building A Scalable Forward Flux Sampling Framework using Big Data and HPC. , 2019, , .		3
8	A generalized deep learning approach for local structure identification in molecular simulations. Chemical Science, 2019, 10, 7503-7515.	7.4	55
9	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
10	Contour forward flux sampling: Sampling rare events along multiple collective variables. Journal of Chemical Physics, 2019, 150, 024103.	3.0	20
11	Surface chemistry effects on heterogeneous clathrate hydrate nucleation: A molecular dynamics study. Journal of Chemical Thermodynamics, 2018, 117, 205-213.	2.0	17
12	Nucleation mechanism of clathrate hydrates of water-soluble guest molecules. Journal of Chemical Physics, 2017, 147, 204503.	3.0	32
13	Mental Rolodexing: Senior Chemistry Majors' Understanding of Chemical and Physical Properties. Journal of Chemical Education, 2015, 92, 415-426.	2.3	45
14	PAMAM Dendrimers and Graphene: Materials for Removing Aromatic Contaminants from Water. Environmental Science & Technology, 2015, 49, 4490-4497.	10.0	40
15	Association of small aromatic molecules with PAMAM dendrimers. Physical Chemistry Chemical Physics, 2015, 17, 29548-29557.	2.8	9
16	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