

Ryan S Defever

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/149047/publications.pdf>

Version: 2024-02-01

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	Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. <i>AIChE Journal</i> , 2021, 67, e17206.	3.6	16
2	MoSDeF Cassandra: A complete Python interface for the Cassandra Monte Carlo software. <i>Journal of Computational Chemistry</i> , 2021, 42, 1321-1331.	3.3	4
3	Machine Learning Directed Optimization of Classical Molecular Modeling Force Fields. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4400-4414.	5.4	29
4	Computing the Liquidus of Binary Monatomic Salt Mixtures with Direct Simulation and Alchemical Free Energy Methods. <i>Journal of Physical Chemistry A</i> , 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. <i>Journal of Chemical Physics</i> , 2020, 153, 214502.	3.0	19
6	Melting points of alkali chlorides evaluated for a polarizable and non-polarizable model. <i>Journal of Chemical Physics</i> , 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. <i>Chemical Science</i> , 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. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2190-2198.	5.4	37
10	Contour forward flux sampling: Sampling rare events along multiple collective variables. <i>Journal of Chemical Physics</i> , 2019, 150, 024103.	3.0	20
11	Surface chemistry effects on heterogeneous clathrate hydrate nucleation: A molecular dynamics study. <i>Journal of Chemical Thermodynamics</i> , 2018, 117, 205-213.	2.0	17
12	Nucleation mechanism of clathrate hydrates of water-soluble guest molecules. <i>Journal of Chemical Physics</i> , 2017, 147, 204503.	3.0	32
13	Mental Rolodexing: Senior Chemistry Majors's™ Understanding of Chemical and Physical Properties. <i>Journal of Chemical Education</i> , 2015, 92, 415-426.	2.3	45
14	PAMAM Dendrimers and Graphene: Materials for Removing Aromatic Contaminants from Water. <i>Environmental Science & Technology</i> , 2015, 49, 4490-4497.	10.0	40
15	Association of small aromatic molecules with PAMAM dendrimers. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25916-25927.	2.8	65