Mangesh I Chaudhari

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/434818/publications.pdf

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19	420	687363 13	752698 20
papers	citations	h-index	g-index

20	20	20	536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Scaling Atomic Partial Charges of Carbonate Solvents for Lithium Ion Solvation and Diffusion. Journal of Chemical Theory and Computation, 2016, 12, 5709-5718.	5.3	64
2	Dielectric Relaxation of Ethylene Carbonate and Propylene Carbonate from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1849-1853.	2.6	42
3	Molecular-scale hydrophobic interactions between hard-sphere reference solutes are attractive and endothermic. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 20557-20562.	7.1	38
4	Octa-Coordination and the Aqueous Ba²⁺ Ion. Journal of Physical Chemistry B, 2015, 119, 8746-8753.	2.6	34
5	Molecular Dynamics of Lithium Ion Transport in a Model Solid Electrolyte Interphase. Scientific Reports, 2018, 8, 10736.	3.3	33
6	The Impact of Protonation on Early Translocation of Anthrax Lethal Factor: Kinetics from Molecular Dynamics Simulations and Milestoning Theory. Journal of the American Chemical Society, 2017, 139, 14837-14840.	13.7	30
7	Molecular Theory and the Effects of Solute Attractive Forces on Hydrophobic Interactions. Journal of Physical Chemistry B, 2016, 120, 1864-1870.	2.6	25
8	Statistical Analyses of Hydrophobic Interactions: A Mini-Review. Journal of Physical Chemistry B, 2016, 120, 6455-6460.	2.6	22
9	Hydration of Kr(aq) in Dilute and Concentrated Solutions. Journal of Physical Chemistry B, 2015, 119, 9098-9102.	2.6	20
10	Strontium and barium in aqueous solution and a potassium channel binding site. Journal of Chemical Physics, 2018, 148, 222831.	3.0	18
11	Utility of chemical computations in predicting solution free energies of metal ions. Molecular Simulation, 2018, 44, 110-116.	2.0	16
12	Interfaces of propylene carbonate. Journal of Chemical Physics, 2013, 138, 114708.	3.0	15
13	Assessment of Simple Models for Molecular Simulation of Ethylene Carbonate and Propylene Carbonate as Solvents for Electrolyte Solutions. Topics in Current Chemistry, 2018, 376, 7.	5.8	15
14	Quasi-chemical theory of Fâ˜(aq): The â€œno split occupancies ruleâ€•revisited. Journal of Chemical Physics, 2017, 147, 161728.	3.0	12
15	Role of Solute Attractive Forces in the Atomic-Scale Theory of Hydrophobic Effects. Journal of Physical Chemistry B, 2018, 122, 6272-6276.	2.6	12
16	Communication: Direct observation of a hydrophobic bond in loop closure of a capped (â€“OCH2CH2â€“)n oligomer in water. Journal of Chemical Physics, 2010, 133, 231102.	3.0	8
17	Molecular Simulation Results on Charged Carbon Nanotube Forestâ€Based Supercapacitors. ChemSusChem, 2018, 11, 1927-1932.	6.8	7
18	Probing Translocation in Mutants of the Anthrax Channel: Atomically Detailed Simulations with Milestoning. Journal of Physical Chemistry B, 2018, 122, 10296-10305.	2.6	6

#	Article	IF	Citations
19	Nanoporous Hydrogels for the Observation of Anthrax Exotoxin Translocation Dynamics. ACS Applied Materials & Interfaces, 2018, 10, 13342-13349.	8.0	2