Arindam Bankura

List of Publications by Year
in descending order

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11	503	1163117	1281871
papers	citations	8	11
		h-index	g-index

11	11	11	746
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A <scp>QM</scp>/<scp>MM</scp> simulation study of transamination reaction at the active site of aspartate aminotransferase: Free energy landscape and proton transfer pathways. Journal of Computational Chemistry, 2020, 41, 2684-2694.	3.3	6
2	A systematic study of chloride ion solvation in water using van der Waals inclusive hybrid density functional theory. Molecular Physics, 2015, 113, 2842-2854.	1.7	47
3	Proton transfer through hydrogen bonds in two-dimensional water layers: A theoretical study based on ab initio and quantum-classical simulations. Journal of Chemical Physics, 2015, 142, 044701.	3.0	20
4	Structure, Dynamics, and Spectral Diffusion of Water from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2014, 118, 29401-29411.	3.1	139
5	Hydration structure of Na⁺and K⁺fromab initiomolecular dynamics based on modern density functional theory. Molecular Physics, 2014, 112, 1448-1456.	1.7	37
6	Hydration structure of salt solutions from ab initio molecular dynamics. Journal of Chemical Physics, 2013, 138, 014501.	3.0	158
7	Hydroxide Ion Can Move Faster Than an Excess Proton through One-Dimensional Water Chains in Hydrophobic Narrow Pores. Journal of Physical Chemistry B, 2012, 116, 9744-9757.	2.6	37
8	A first principles molecular dynamics study of the solvation structure and migration kinetics of an excess proton and a hydroxide ion in binary water-ammonia mixtures. Journal of Chemical Physics, 2012, 136, 114509.	3.0	8
9	Hydration structure and dynamics of a hydroxide ion in water clusters of varying size and temperature: Quantum chemical and ab initio molecular dynamics studies. Chemical Physics, 2012, 400, 154-164.	1.9	27
10	A first principles theoretical study of the hydration structure and dynamics of an excess proton in water clusters of varying size and temperature. Chemical Physics, 2011, 387, 92-102.	1.9	19
11	Hydration and translocation of an excess proton in water clusters: Anab initio molecular dynamics study. Pramana - Journal of Physics, 2005, 65, 763-768.	1.8	5