Debashree Chakraborty

List of Publications by Year
in descending order

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31 papers	520 citations	759233 12 h-index	677142 22 g-index
31 all docs	31 docs citations	31 times ranked	553 citing authors

#	Article	IF	Citations
1	How Crystals Nucleate and Grow in Aqueous NaCl Solution. Journal of Physical Chemistry Letters, 2013, 4, 573-578.	4.6	85
2	Evidence that crystal nucleation in aqueous NaCl solution Occurs by the two-step mechanism. Chemical Physics Letters, 2013, 587, 25-29.	2.6	53
3	Effects of ion concentration on the hydrogen bonded structure of water in the vicinity of ions in aqueous NaCl solutions. Journal of Chemical Sciences, 2008, 120, 71-77.	1.5	39
4	A first principles simulation study of fluctuations of hydrogen bonds and vibrational frequencies of water at liquidâ€“vapor interface. Chemical Physics, 2012, 392, 96-104.	1.9	39
5	Hydrogen bonded structure and dynamics of liquid-vapor interface of water-ammonia mixture: An ab initio molecular dynamics study. Journal of Chemical Physics, 2011, 135, 114510.	3.0	38
6	An analysis of voids and necks in supercritical water. Journal of Molecular Liquids, 2011, 163, 1-6.	4.9	24
7	Interstitial Voids and Resultant Density of Liquid Water: A First-Principles Molecular Dynamics Study. ACS Omega, 2018, 3, 2010-2017.	3.5	23
8	Stay Wet, Stay Stable? How Internal Water Helps the Stability of Thermophilic Proteins. Journal of Physical Chemistry B, 2015, 119, 12760-12770.	2.6	21
9	Structural and Thermophysical Anomalies of Liquid Water: A Tale of Molecules in the Instantaneous Low- and High-Density Regions. Journal of Physical Chemistry B, 2020, 124, 1071-1081.	2.6	20
10	Diffusion of ions in supercritical water: Dependence on ion size and solvent density and roles of voids and necks. Journal of Molecular Liquids, 2011, 162, 12-19.	4.9	19
11	Anti-corrosion investigation of a new nitro veratraldehyde substituted imidazopyridine derivative Schiff base on mild steel surface in hydrochloric acid medium: Experimental, computational, surface morphological analysis. Materials Chemistry and Physics, 2022, 281, 125855.	4.0	17
12	Effective inhibition of mild steel corrosion by 6-bromo-(2,4-dimethoxyphenyl)methylidene]imidazo [1,2-a]pyridine-2-carbohydrazide in 0.5ÂM HCl: Insights from experimental and computational study. Journal of Molecular Structure, 2021, 1232, 130074.	3.6	15
13	Effect of hydrophobic and hydrogen bonding interactions on the potency of ÃŸâ€alanine analogs of Gâ€protein coupled glucagon receptor inhibitors. Proteins: Structure, Function and Bioinformatics, 2020, 88, 327-344.	2.6	14
14	Computational insights into factor affecting the potency of diaryl sulfone analogs as Escherichia coli dihydropteroate synthase inhibitors. Computational Biology and Chemistry, 2019, 78, 37-52.	2.3	12
15	Epitope-Based Potential Vaccine Candidate for Humoral and Cell-Mediated Immunity to Combat Severe Acute Respiratory Syndrome Coronavirus 2 Pandemic. Journal of Physical Chemistry Letters, 2020, 11, 9920-9930.	4.6	12
16	Pressure effects on diffusion in liquid ammonia : A simulation study using a combination of isobaric-isothermal and microcanonical molecular dynamics. Indian Journal of Physics, 2009, 83, 91-100.	1.8	11
17	Carbohelicenes and thiahelicene from phthalaldehydes through Perkin approach. Journal of Molecular Structure, 2019, 1195, 309-314.	3.6	10
18	Voids and necks in liquid ammonia and their roles in diffusion of ions of varying size. Journal of Computational Chemistry, 2012, 33, 843-852.	3.3	8

#	Article	IF	Citations
19	Effect of cosolvents in the preferential binding affinity of water in aqueous solutions of amino acids and amides. Journal of Molecular Liquids, 2020, 300, 112375.	4.9	8
20	Hydrophilicity of the hydrophobic group: Effect of cosolvents and ions. Journal of Molecular Liquids, 2019, 280, 389-398.	4.9	7
21	Structural and dynamical properties of water in surfactant-like peptide-based nanotubes: Effect of pore size, tube length and charge. Journal of Molecular Liquids, 2021, 323, 115033.	4.9	7
22	In-silico epitope identification and design of Uricase mutein with reduced immunogenicity. Process Biochemistry, 2020, 92, 288-302.	3.7	6
23	Theoretical insights into molecular mechanism and energy criteria of PARPâ€2 enzyme inhibition by benzimidazole analogues. Proteins: Structure, Function and Bioinformatics, 2021, 89, 988-1004.	2.6	6
24	Molecular mechanism of inhibition of COVID-19 main protease by Î²-adrenoceptor agonists and adenosine deaminase inhibitors using in silico methods. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5112-5127.	3.5	5
25	Preferential binding affinity of ions and their effect on structure and dynamics of water near antimicrobial peptide. Journal of Molecular Liquids, 2021, 344, 117789.	4.9	5
26	Exploring the potential role of quercetin in corrosion inhibition of aluminium alloy 6063 in hydrochloric acid solution by experimental and theoretical studies. Journal of Adhesion Science and Technology, 2022, 36, 2020-2045.	2.6	5
27	Temperature-Dependent Conformational Evolution of SARS CoV-2 RNA Genome Using Network Analysis. Journal of Physical Chemistry B, 2021, 125, 10672-10681.	2.6	3
28	Deciphering the competitive inhibition of dihydropteroate synthase by 8 marcaptoguanine analogs: enhanced potency in phenylsulfonyl fragments. Journal of Biomolecular Structure and Dynamics, 2021, , 1-20.	3.5	3
29	Influence of Ion Specificity and Concentration on the Conformational Transition of Intrinsically Disordered Sheep Prion Peptide. ChemPhysChem, 2022, 23, .	2.1	3
30	Diverse interactions of aggregated insulin with selected coumarin dyes: Time dependent fluorogenicity, simulation studies and comparison with thioflavin T. Dyes and Pigments, 2021, 184, 108796.	3.7	1
31	Exploring the multiple conformational states of RNA genome through interhelical dynamics and network analysis. Journal of Molecular Graphics and Modelling, 2022, 116, 108264.	2.4	1