Suman Chakrabarty

List of Publications by Year
in descending order

55 papers	1,302 citations	279798 23 h-index	377865 34 g-index
56 all docs	56 docs citations	56 times ranked	1906 citing authors

#	Article	IF	Citations
1	Effect of the amino acid l-histidine on methane hydrate growth kinetics. Journal of Natural Gas Science and Engineering, 2016, 35, 1453-1462.	4.4	114
2	Hidden electrostatic basis of dynamic allostery in a PDZ domain. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5825-E5834.	7.1	78
3	Correlating Nitrile IR Frequencies to Local Electrostatics Quantifies Noncovalent Interactions of Peptides and Proteins. Journal of Physical Chemistry B, 2016, 120, 4034-4046.	2.6	75
4	Quantifying the Mechanism of Phosphate Monoester Hydrolysis in Aqueous Solution by Evaluating the Relevant Ab Initio QM/MM Free-Energy Surfaces. Journal of Physical Chemistry B, 2013, 117, 12807-12819.	2.6	47
5	Effect of Sodium Dodecyl Sulfate Surfactant on Methane Hydrate Formation: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 6536-6542.	2.6	47
6	Elucidating the Mechanism of Nucleation near the Gas-Liquid Spinodal. Physical Review Letters, 2007, 98, 206104.	7.8	46
7	Exploration of the cytochrome c oxidase pathway puzzle and examination of the origin of elusive mutational effects. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 413-426.	1.0	42
8	Capturing the energetics of water insertion in biological systems: The water flooding approach. Proteins: Structure, Function and Bioinformatics, 2013, 81, 93-106.	2.6	41
9	Critical Assessment of the Interaction between DNA and Choline Amino Acid Ionic Liquids: Evidences of Multimodal Binding and Stability Enhancement. ACS Central Science, 2018, 4, 1642-1651.	11.3	40
10	Amino-Acid-Based Ionic Liquids for the Improvement in Stability and Activity of Cytochrome c: A Combined Experimental and Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 10100-10109.	2.6	38
11	Anomalous Behavior of Linear Hydrocarbon Chains in Waterâ€“DMSO Binary Mixture at Low DMSO Concentration. Journal of Physical Chemistry B, 2011, 115, 7612-7620.	2.6	37
12	Bioactive Polymersomes Self-Assembled from Amphiphilic PPO-GlycoPolypeptides: Synthesis, Characterization, and Dual-Dye Encapsulation. Langmuir, 2015, 31, 3402-3412.	3.5	34
13	Structural Order of Water Molecules around Hydrophobic Solutes: Length-Scale Dependence and Soluteâ€“Solvent Coupling. Journal of Physical Chemistry B, 2015, 119, 11346-11357.	2.6	33
14	Mechanism of Unfolding of Human Prion Protein. Journal of Physical Chemistry B, 2017, 121, 550-564.	2.6	33
15	Realistic simulation of the activation of voltage-gated ion channels. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 3335-3340.	7.1	32
16	Two-Dimensional Infrared Spectroscopy Reveals Cosolvent-Composition-Dependent Crossover in Intermolecular Hydrogen-Bond Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 1604-1609.	4.6	32
17	Proton-transport mechanisms in cytochrome c oxidase revealed by studies of kinetic isotope effects. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 1083-1094.	1.0	31
18	Temperature-Induced Misfolding in Prion Protein: Evidence of Multiple Partially Disordered States Stabilized by Non-Native Hydrogen Bonds. Biochemistry, 2017, 56, 833-844.	2.5	30

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19	Coarse grained model for exploring voltage dependent ion channels. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 303-317.	2.6	28
20	Self-Organization of n-Alkane Chains in Water: Length Dependent Crossover from Helix and Toroid to Molten Globule. Journal of Physical Chemistry B, 2009, 113, 8446-8448.	2.6	27
21	Universal Power Law in the Orientational Relaxation in Thermotropic Liquid Crystals. Physical Review Letters, 2005, 95, 197801.	7.8	26
22	Exploration of the presence of bulk-like water in AOT reverse micelles and water-in-oil nanodroplets: the role of charged interfaces, confinement size and properties of water. Physical Chemistry Chemical Physics, 2016, 18, 21767-21779.	2.8	26
23	A comparison of different water models for melting point calculation of methane hydrate using molecular dynamics simulations. Chemical Physics, 2019, 516, 6-14.	1.9	25
24	Effect of Solvation on Electron Detachment and Excitation Energies of a Green Fluorescent Protein Chromophore Variant. Journal of Physical Chemistry B, 2016, 120, 4410-4420.	2.6	21
25	Charge transfer liquid: a stable donorâ€“acceptor interaction in the solvent-free liquid state. Chemical Communications, 2019, 55, 9371-9374.	4.1	20
26	Gas-liquid nucleation in a two dimensional system. Journal of Chemical Physics, 2008, 129, 234704.	3.0	19
27	Interplay between crystallization and glass transition in binary Lennard-Jones mixtures. Journal of Chemical Physics, 2013, 139, 104501.	3.0	18
28	Nucleotide Dependent Switching in Rho GTPase: Conformational Heterogeneity and Competing Molecular Interactions. Scientific Reports, 2017, 7, 45829.	3.3	18
29	Molecular View of CO2 Capture by Polyethylenimine: Role of Structural and Dynamical Heterogeneity. Langmuir, 2018, 34, 5138-5148.	3.5	18
30	Molecular Dynamics Simulation and Experimental Study on the Growth of Methane Hydrate in Presence of Methanol and Sodium Chloride. Energy Procedia, 2017, 105, 5026-5033.	1.8	16
31	Organoselenium Compounds as Acetylcholinesterase Inhibitors: Evidence and Mechanism of Mixed Inhibition. Journal of Physical Chemistry B, 2021, 125, 1531-1541.	2.6	16
32	Macro and Molecular Level Insights on Gas Hydrate Growth in the Presence of Hofmeister Salts. Industrial & Engineering Chemistry Research, 2020, 59, 20591-20600.	3.7	16
33	Partially bioâ€based poly(amide imide)s by polycondensation of aromatic diacylhydrazides based on lignināderived phenolic acids and aromatic dianhydrides: Synthesis, characterization, and computational studies. Journal of Polymer Science Part A, 2017, 55, 3636-3645.	2.3	15
34	Modeling gating charge and voltage changes in response to charge separation in membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11353-11358.	7.1	13
35	Sulfonylurea Class of Antidiabetic Drugs Inhibit Acetylcholinesterase Activity: Unexplored Auxiliary Pharmacological Benefit toward Alzheimerâ€™s Disease. ACS Pharmacology and Translational Science, 2021, 4, 193-205.	4.9	13
36	Replica Exchange Molecular Dynamics Study of Dimerization in Prion Protein: Multiple Modes of Interaction and Stabilization. Journal of Physical Chemistry B, 2016, 120, 7332-7345.	2.6	12

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37	Protonation-Induced Dynamic Allostery in PDZ Domain: Evidence of Perturbation-Independent Universal Response Network. Journal of Physical Chemistry Letters, 2020, 11, 9026-9031.	4.6	12
38	Composition dependence of the glass forming ability in binary mixtures: The role of demixing entropy. Journal of Chemical Physics, 2016, 145, 034503.	3.0	11
39	Power law relaxation and glassy dynamics in Lebwohl-Lasher model near the isotropic-nematic phase transition. Physical Review E, 2006, 73, 061706.	2.1	10
40	Origin of Unusually High Fluorescence Anisotropy of 3-Hydroxyflavone in Water: Formation of Probeâ€“Solvent Cage-like Cluster. Journal of Physical Chemistry B, 2020, 124, 173-180.	2.6	10
41	Morphology and dynamics of self-assembled structures in mixed surfactant systems (SDSÂ+ÂCAPB) in the context of methane hydrate growth. Journal of Molecular Liquids, 2020, 319, 114296.	4.9	10
42	Heterogeneous nucleation in citrate synthesis of AgNPs: Effect of mixing and solvation dynamics. Chemical Engineering Journal, 2021, 421, 127753.	12.7	10
43	Size-Dependent Orderâ€“Disorder Crossover in Hydrophobic Hydration: Comparison between Spherical Solutes and Linear Alcohols. ACS Omega, 2022, 7, 2671-2678.	3.5	9
44	How Far Is â€œBulk Waterâ€•from Interfaces? Depends on the Nature of the Surface and What We Measure. Journal of Physical Chemistry B, 2022, 126, 1125-1135.	2.6	9
45	Chakrabarty, Santra, and Bagchi Reply:. Physical Review Letters, 2008, 101, .	7.8	8
46	Electrostatic Origin of the Red Solvatochromic Shift of DFHBDI in RNA Spinach. Journal of Physical Chemistry B, 2017, 121, 4790-4798.	2.6	8
47	Soluble polybenzimidazoles with intrinsic porosity: Synthesis, structure, properties and processability. Journal of Polymer Science Part A, 2018, 56, 1046-1057.	2.3	7
48	Molecular Insight into Dyeâ€“Surfactant Interaction at Premicellar Concentrations: A Combined Two-Photon Absorption and Molecular Dynamics Simulation Study. Langmuir, 2022, 38, 3105-3112.	3.5	7
49	Temperature dependent free energy surface of polymer folding from equilibrium and quench studies. Journal of Chemical Physics, 2010, 133, 214901.	3.0	4
50	Hydroxyl Group-Directed Solvation of Excited-State Intramolecular Proton Transfer Probes in Water: A Demonstration from the Fluorescence Anisotropy of Hydroxyflavones. Journal of Physical Chemistry A, 2021, 125, 57-64.	2.5	4
51	Support Vector Regression-Based Monte Carlo Simulation of Flexible Water Clusters. ACS Omega, 2020, 5, 7065-7073.	3.5	2
52	Structural and dynamical heterogeneity of water trapped inside Na+-pumping KR2 rhodopsin in the dark state. Journal of Chemical Physics, 2021, 154, 215101.	3.0	2
53	Probing into Methylene Blue Interaction with Polyglutamic Acid: Spectroscopic and Molecular Dynamics Simulation Studies. Asian Journal of Chemistry, 2019, 31, 1949-1958.	0.3	1
54	A Thermodynamic View of Dynamic Allostery in a PDZ Domain Protein. Biophysical Journal, 2019, 116, 163a.	0.5	1

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55	Role of Buried Water in the Mechanism of Photoactivation of KR2 Rhodopsin. Biophysical Journal, 2021, 120, 131a.	0.5	0