Jagannath Mondal

List of Publications by Year
in descending order

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59 papers	1,511 citations	361413 20 h-index	361022 35 g-index
67 all docs	67 docs citations	67 times ranked	1847 citing authors

#	Article	IF	Citations
1	Mechanism of Coordinated Gating and Signal Transduction in Purine Biosynthetic Enzyme Formylglycinamidine Synthetase. ACS Catalysis, 2022, 12, 1930-1944.	11.2	5
2	Solventâ€™s Role in Cavityâ€“Ligand Recognition Would Depend on the Mode of Ligand Diffusion. Journal of Physical Chemistry B, 2022, 126, 2952-2958.	2.6	1
3	Hi-C embedded polymer model of Escherichia coli reveals the origin of heterogeneous subdiffusion in chromosomal loci. Physical Review E, 2022, 105, .	2.1	6
4	DNA-Functionalized Gold Nanorods for Perioperative Optical Imaging and Photothermal Therapy of Triple-Negative Breast Cancer. ACS Applied Nano Materials, 2022, 5, 9159-9169.	5.0	10
5	Zwitterionic Osmolytes Revive Surface Charges under Salt Stress via Dual Mechanisms. Journal of Physical Chemistry Letters, 2022, 13, 5660-5668.	4.6	4
6	A Hiâ€“C data-integrated model elucidatesE. colichromosomeâ€™s multiscale organization at various replication stages. Nucleic Acids Research, 2021, 49, 3077-3091.	14.5	18
7	Reconciling conformational heterogeneity and substrate recognition in cytochrome P450. Biophysical Journal, 2021, 120, 1732-1745.	0.5	7
8	Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly. Journal of Physical Chemistry B, 2021, 125, 5285-5295.	2.6	4
9	Mechanistic Insights on ATPâ€™s Role as a Hydrotrope. Journal of Physical Chemistry B, 2021, 125, 7717-7731.	2.6	21
10	Spontaneous transmembrane pore formation by short-chain synthetic peptide. Biophysical Journal, 2021, 120, 4557-4574.	0.5	6
11	A deep autoencoder framework for discovery of metastable ensembles in biomacromolecules. Journal of Chemical Physics, 2021, 155, 114106.	3.0	14
12	Mechanistic underpinning of cell aspect ratio-dependent emergent collective motions in swarming bacteria. Soft Matter, 2021, 17, 7322-7331.	2.7	10
13	An Appraisal of Computer Simulation Approaches in Elucidating Biomolecular Recognition Pathways. Journal of Physical Chemistry Letters, 2021, 12, 633-641.	4.6	12
14	Elucidating the Mechanism of Nitrogen Doping in Graphene Oxide: Structural Evolution of Dopants and the Role of Oxygen. Journal of Physical Chemistry C, 2021, 125, 22547-22553.	3.1	3
15	Molecular dynamics simulations elucidate oligosaccharide recognition pathways by galectin-3 at atomic resolution. Journal of Biological Chemistry, 2021, 297, 101271.	3.4	3
16	Role of molecular dynamics in optimising ligand discovery: Case study with novel inhibitor search for peptidyl t-RNA hydrolase. Chemical Physics Impact, 2021, 3, 100048.	3.5	3
17	Bottom-Up View of the Mechanism of Action of Protein-Stabilizing Osmolytes. Journal of Physical Chemistry B, 2020, 124, 11316-11323.	2.6	10
18	Unifying the Contrasting Mechanisms of Protein-Stabilizing Osmolytes. Journal of Physical Chemistry B, 2020, 124, 6565-6574.	2.6	26

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19	Nonaffine Displacements Encode Collective Conformational Fluctuations in Proteins. Journal of Chemical Theory and Computation, 2020, 16, 2508-2516.	5.3	6
20	Capturing Proteinâ€“Ligand Recognition Pathways in Coarse-Grained Simulation. Journal of Physical Chemistry Letters, 2020, 11, 5302-5311.	4.6	28
21	Structural evolution of BCN systems from graphene oxide towards electrocatalytically active atomic layers. Materials Chemistry Frontiers, 2020, 4, 2330-2338.	5.9	11
22	Engineering the hydrogen evolution reaction of transition metals: effect of Li ions. Journal of Materials Chemistry A, 2020, 8, 15795-15808.	10.3	14
23	On the role of solvent in hydrophobic cavityâ€“ligand recognition kinetics. Journal of Chemical Physics, 2020, 152, 074104.	3.0	7
24	Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation. Science Advances, 2020, 6, eaay7919.	10.3	10
25	Membrane-Disrupting Nanofibrous Peptide Hydrogels. ACS Biomaterials Science and Engineering, 2019, 5, 4657-4670.	5.2	38
26	In Silico Reoptimization of Binding Affinity and Drug-Resistance Circumvention Ability in Kinase Inhibitors: A Case Study with RL-45 and Src Kinase. Journal of Physical Chemistry B, 2019, 123, 6664-6672.	2.6	9
27	Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. Journal of Physical Chemistry C, 2019, 123, 17249-17254.	3.1	6
28	Osmolyte-Induced Macromolecular Aggregation Is Length-Scale Dependent. Journal of Physical Chemistry B, 2019, 123, 8697-8703.	2.6	8
29	Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 6203-6212.	5.3	15
30	Osmolyte-Induced Collapse of a Charged Macromolecule. Journal of Physical Chemistry B, 2019, 123, 4636-4644.	2.6	12
31	Role of Î± and Î² relaxations in collapsing dynamics of a polymer chain in supercooled glass-forming liquid. Journal of Chemical Physics, 2019, 150, 114503.	3.0	4
32	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. PLoS Computational Biology, 2019, 15, e1006665.	3.2	11
33	A brief appraisal of computational modeling of antimicrobial peptidesâ€™ activity. Drug Development Research, 2019, 80, 28-32.	2.9	12
34	Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 10034-10041.	3.1	18
35	On the hydrogen evolution reaction activity of grapheneâ€“hBN van der Waals heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 15007-15014.	2.8	41
36	Mapping the Substrate Recognition Pathway in Cytochrome P450. Journal of the American Chemical Society, 2018, 140, 17743-17752.	13.7	42

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37	Assessment and optimization of collective variables for protein conformational landscape: GB1 Î²-hairpin as a case study. Journal of Chemical Physics, 2018, 149, 094101.	3.0	26
38	Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme. PLoS Computational Biology, 2018, 14, e1006180.	3.2	58
39	Heterogeneous Impacts of Protein-Stabilizing Osmolytes on Hydrophobic Interaction. Journal of Physical Chemistry B, 2018, 122, 6922-6930.	2.6	22
40	How and when does an anticancer drug leave its binding site?. Science Advances, 2017, 3, e1700014.	10.3	111
41	How Does a Hydrophobic Macromolecule Respond to a Mixed Osmolyte Environment?. Journal of Physical Chemistry B, 2016, 120, 10969-10978.	2.6	16
42	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. Journal of the American Chemical Society, 2016, 138, 2472-2475.	13.7	34
43	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. Journal of the American Chemical Society, 2016, 138, 4608-4615.	13.7	44
44	How osmolytes influence hydrophobic polymer conformations: A unified view from experiment and theory. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 9270-9275.	7.1	98
45	Mechanically-driven phase separation in a growing bacterial colony. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2166-73.	7.1	95
46	Role of water and steric constraints in the kinetics of cavityâ€“ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019.	7.1	74
47	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. Journal of Chemical Theory and Computation, 2014, 10, 5696-5705.	5.3	61
48	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. Macromolecules, 2014, 47, 438-446.	4.8	50
49	Self-Assembly of Gemini Surfactants: A Computer Simulation Study. Journal of Physical Chemistry B, 2013, 117, 4254-4262.	2.6	44
50	When Does Trimethylamine N-Oxide Fold a Polymer Chain and Urea Unfold It?. Journal of Physical Chemistry B, 2013, 117, 8723-8732.	2.6	99
51	How hydrophobic drying forces impact the kinetics of molecular recognition. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13277-13282.	7.1	45
52	Effect of secondary structure on the self-assembly of amphiphilic molecules: A multiscale simulation study. Journal of Chemical Physics, 2012, 136, 084902.	3.0	13
53	Sequence-Dependent pK_aShift Induced by Molecular Self-Assembly: Insights from Computer Simulation. Journal of Physical Chemistry B, 2012, 116, 491-495.	2.6	4
54	Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in E.Âcoli Cells. Biophysical Journal, 2011, 100, 2605-2613.	0.5	96

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55	Sequence dependent self-assembly of Î²-peptides: Insights from a coarse-grained model. Journal of Chemical Physics, 2010, 132, 065103.	3.0	11
56	Self-Assembly of Î²-Peptides: Insight from the Pair and Many-Body Free Energy of Association. Journal of Physical Chemistry C, 2010, 114, 13551-13556.	3.1	11
57	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	2.6	31
58	Sequence-Directed Organization of Î²-Peptides in Self-Assembled Monolayers. Journal of Physical Chemistry B, 2009, 113, 9379-9385.	2.6	9
59	Impact of Inert Crowders on Hostâ€“Guest Recognition Process. Journal of Physical Chemistry B, 0, , .	2.6	3