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	How and when does an anticancer drug leave its binding site?. Science Advances, 2017, 3, e1700014.	10.3	111
2	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
3	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
4	Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in E.Âcoli Cells. Biophysical Journal, 2011, 100, 2605-2613.	0.5	96
5	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
6	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
7	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
8	Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme. PLoS Computational Biology, 2018, 14, e1006180.	3.2	58
9	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. Macromolecules, 2014, 47, 438-446.	4.8	50
10	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
11	Self-Assembly of Gemini Surfactants: A Computer Simulation Study. Journal of Physical Chemistry B, 2013, 117, 4254-4262.	2.6	44
12	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. Journal of the American Chemical Society, 2016, 138, 4608-4615.	13.7	44
13	Mapping the Substrate Recognition Pathway in Cytochrome P450. Journal of the American Chemical Society, 2018, 140, 17743-17752.	13.7	42
14	On the hydrogen evolution reaction activity of grapheneâ€“hBN van der Waals heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 15007-15014.	2.8	41
15	Membrane-Disrupting Nanofibrous Peptide Hydrogels. ACS Biomaterials Science and Engineering, 2019, 5, 4657-4670.	5.2	38
16	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. Journal of the American Chemical Society, 2016, 138, 2472-2475.	13.7	34
17	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	2.6	31
18	Capturing Proteinâ€“Ligand Recognition Pathways in Coarse-Grained Simulation. Journal of Physical Chemistry Letters, 2020, 11, 5302-5311.	4.6	28

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19	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
20	Unifying the Contrasting Mechanisms of Protein-Stabilizing Osmolytes. Journal of Physical Chemistry B, 2020, 124, 6565-6574.	2.6	26
21	Heterogeneous Impacts of Protein-Stabilizing Osmolytes on Hydrophobic Interaction. Journal of Physical Chemistry B, 2018, 122, 6922-6930.	2.6	22
22	Mechanistic Insights on ATPâ€™s Role as a Hydrotrope. Journal of Physical Chemistry B, 2021, 125, 7717-7731.	2.6	21
23	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
24	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
25	How Does a Hydrophobic Macromolecule Respond to a Mixed Osmolyte Environment?. Journal of Physical Chemistry B, 2016, 120, 10969-10978.	2.6	16
26	Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 6203-6212.	5.3	15
27	Engineering the hydrogen evolution reaction of transition metals: effect of Li ions. Journal of Materials Chemistry A, 2020, 8, 15795-15808.	10.3	14
28	A deep autoencoder framework for discovery of metastable ensembles in biomacromolecules. Journal of Chemical Physics, 2021, 155, 114106.	3.0	14
29	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
30	Osmolyte-Induced Collapse of a Charged Macromolecule. Journal of Physical Chemistry B, 2019, 123, 4636-4644.	2.6	12
31	A brief appraisal of computational modeling of antimicrobial peptidesâ€™ activity. Drug Development Research, 2019, 80, 28-32.	2.9	12
32	An Appraisal of Computer Simulation Approaches in Elucidating Biomolecular Recognition Pathways. Journal of Physical Chemistry Letters, 2021, 12, 633-641.	4.6	12
33	Sequence dependent self-assembly of Î²-peptides: Insights from a coarse-grained model. Journal of Chemical Physics, 2010, 132, 065103.	3.0	11
34	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
35	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. PLoS Computational Biology, 2019, 15, e1006665.	3.2	11
36	Structural evolution of BCN systems from graphene oxide towards electrocatalytically active atomic layers. Materials Chemistry Frontiers, 2020, 4, 2330-2338.	5.9	11

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37	Bottom-Up View of the Mechanism of Action of Protein-Stabilizing Osmolytes. Journal of Physical Chemistry B, 2020, 124, 11316-11323.	2.6	10
38	Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation. Science Advances, 2020, 6, eaay7919.	10.3	10
39	Mechanistic underpinning of cell aspect ratio-dependent emergent collective motions in swarming bacteria. Soft Matter, 2021, 17, 7322-7331.	2.7	10
40	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
41	Sequence-Directed Organization of Î²-Peptides in Self-Assembled Monolayers. Journal of Physical Chemistry B, 2009, 113, 9379-9385.	2.6	9
42	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
43	Osmolyte-Induced Macromolecular Aggregation Is Length-Scale Dependent. Journal of Physical Chemistry B, 2019, 123, 8697-8703.	2.6	8
44	On the role of solvent in hydrophobic cavityâ€“ligand recognition kinetics. Journal of Chemical Physics, 2020, 152, 074104.	3.0	7
45	Reconciling conformational heterogeneity and substrate recognition in cytochrome P450. Biophysical Journal, 2021, 120, 1732-1745.	0.5	7
46	Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. Journal of Physical Chemistry C, 2019, 123, 17249-17254.	3.1	6
47	Nonaffine Displacements Encode Collective Conformational Fluctuations in Proteins. Journal of Chemical Theory and Computation, 2020, 16, 2508-2516.	5.3	6
48	Spontaneous transmembrane pore formation by short-chain synthetic peptide. Biophysical Journal, 2021, 120, 4557-4574.	0.5	6
49	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
50	Mechanism of Coordinated Gating and Signal Transduction in Purine Biosynthetic Enzyme Formylglycinamidine Synthetase. ACS Catalysis, 2022, 12, 1930-1944.	11.2	5
51	Sequence-Dependent pK_a Shift Induced by Molecular Self-Assembly: Insights from Computer Simulation. Journal of Physical Chemistry B, 2012, 116, 491-495.	2.6	4
52	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
53	Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly. Journal of Physical Chemistry B, 2021, 125, 5285-5295.	2.6	4
54	Zwitterionic Osmolytes Revive Surface Charges under Salt Stress via Dual Mechanisms. Journal of Physical Chemistry Letters, 2022, 13, 5660-5668.	4.6	4

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55	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
56	Molecular dynamics simulations elucidate oligosaccharide recognition pathways by galectin-3 at atomic resolution. Journal of Biological Chemistry, 2021, 297, 101271.	3.4	3
57	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
58	Impact of Inert Crowders on Hostâ€“Guest Recognition Process. Journal of Physical Chemistry B, 0, , .	2.6	3
59	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