

Jagannath Mondal

List of Publications by Year in descending order

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Version: 2024-02-01

59
papers

1,511
citations

361045

20
h-index

360668

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?. <i>Science Advances</i> , 2017, 3, e1700014.	4.7	111
2	When Does Trimethylamine <i>N</i> -Oxide Fold a Polymer Chain and Urea Unfold It?. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8723-8732.	1.2	99
3	How osmolytes influence hydrophobic polymer conformations: A unified view from experiment and theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 9270-9275.	3.3	98
4	Entropy-Based Mechanism of Ribosome-Nucleoid Segregation in <i>E. coli</i> Cells. <i>Biophysical Journal</i> , 2011, 100, 2605-2613.	0.2	96
5	Mechanically-driven phase separation in a growing bacterial colony. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E2166-73.	3.3	95
6	Role of water and steric constraints in the kinetics of cavity-ligand unbinding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 12015-12019.	3.3	74
7	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5696-5705.	2.3	61
8	Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme. <i>PLoS Computational Biology</i> , 2018, 14, e1006180.	1.5	58
9	Atomistic Simulations of Poly(ethylene oxide) in Water and an Ionic Liquid at Room Temperature. <i>Macromolecules</i> , 2014, 47, 438-446.	2.2	50
10	How hydrophobic drying forces impact the kinetics of molecular recognition. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 13277-13282.	3.3	45
11	Self-Assembly of Gemini Surfactants: A Computer Simulation Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4254-4262.	1.2	44
12	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. <i>Journal of the American Chemical Society</i> , 2016, 138, 4608-4615.	6.6	44
13	Mapping the Substrate Recognition Pathway in Cytochrome P450. <i>Journal of the American Chemical Society</i> , 2018, 140, 17743-17752.	6.6	42
14	On the hydrogen evolution reaction activity of graphene-hBN van der Waals heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 15007-15014.	1.3	41
15	Membrane-Disrupting Nanofibrous Peptide Hydrogels. <i>ACS Biomaterials Science and Engineering</i> , 2019, 5, 4657-4670.	2.6	38
16	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. <i>Journal of the American Chemical Society</i> , 2016, 138, 2472-2475.	6.6	34
17	Sequence-Dependent Interaction of β^2 -Peptides with Membranes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13585-13592.	1.2	31
18	Capturing Protein-Ligand Recognition Pathways in Coarse-Grained Simulation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5302-5311.	2.1	28

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19	Assessment and optimization of collective variables for protein conformational landscape: GB1 α -hairpin as a case study. <i>Journal of Chemical Physics</i> , 2018, 149, 094101.	1.2	26
20	Unifying the Contrasting Mechanisms of Protein-Stabilizing Osmolytes. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6565-6574.	1.2	26
21	Heterogeneous Impacts of Protein-Stabilizing Osmolytes on Hydrophobic Interaction. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6922-6930.	1.2	22
22	Mechanistic Insights on ATP's Role as a Hydrotrope. <i>Journal of Physical Chemistry B</i> , 2021, 125, 7717-7731.	1.2	21
23	Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10034-10041.	1.5	18
24	A Hi-C data-integrated model elucidates <i>E. coli</i> chromosome's multiscale organization at various replication stages. <i>Nucleic Acids Research</i> , 2021, 49, 3077-3091.	6.5	18
25	How Does a Hydrophobic Macromolecule Respond to a Mixed Osmolyte Environment?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 10969-10978.	1.2	16
26	Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6203-6212.	2.3	15
27	Engineering the hydrogen evolution reaction of transition metals: effect of Li ions. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15795-15808.	5.2	14
28	A deep autoencoder framework for discovery of metastable ensembles in biomacromolecules. <i>Journal of Chemical Physics</i> , 2021, 155, 114106.	1.2	14
29	Effect of secondary structure on the self-assembly of amphiphilic molecules: A multiscale simulation study. <i>Journal of Chemical Physics</i> , 2012, 136, 084902.	1.2	13
30	Osmolyte-Induced Collapse of a Charged Macromolecule. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4636-4644.	1.2	12
31	A brief appraisal of computational modeling of antimicrobial peptides' activity. <i>Drug Development Research</i> , 2019, 80, 28-32.	1.4	12
32	An Appraisal of Computer Simulation Approaches in Elucidating Biomolecular Recognition Pathways. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 633-641.	2.1	12
33	Sequence dependent self-assembly of α -peptides: Insights from a coarse-grained model. <i>Journal of Chemical Physics</i> , 2010, 132, 065103.	1.2	11
34	Self-Assembly of α -Peptides: Insight from the Pair and Many-Body Free Energy of Association. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13551-13556.	1.5	11
35	On identifying collective displacements in apo-proteins that reveal eventual binding pathways. <i>PLoS Computational Biology</i> , 2019, 15, e1006665.	1.5	11
36	Structural evolution of BCN systems from graphene oxide towards electrocatalytically active atomic layers. <i>Materials Chemistry Frontiers</i> , 2020, 4, 2330-2338.	3.2	11

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37	Bottom-Up View of the Mechanism of Action of Protein-Stabilizing Osmolytes. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11316-11323.	1.2	10
38	Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation. <i>Science Advances</i> , 2020, 6, eaay7919.	4.7	10
39	Mechanistic underpinning of cell aspect ratio-dependent emergent collective motions in swarming bacteria. <i>Soft Matter</i> , 2021, 17, 7322-7331.	1.2	10
40	DNA-Functionalized Gold Nanorods for Perioperative Optical Imaging and Photothermal Therapy of Triple-Negative Breast Cancer. <i>ACS Applied Nano Materials</i> , 2022, 5, 9159-9169.	2.4	10
41	Sequence-Directed Organization of β^2 -Peptides in Self-Assembled Monolayers. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9379-9385.	1.2	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. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6664-6672.	1.2	9
43	Osmolyte-Induced Macromolecular Aggregation Is Length-Scale Dependent. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8697-8703.	1.2	8
44	On the role of solvent in hydrophobic cavity ligand recognition kinetics. <i>Journal of Chemical Physics</i> , 2020, 152, 074104.	1.2	7
45	Reconciling conformational heterogeneity and substrate recognition in cytochrome P450. <i>Biophysical Journal</i> , 2021, 120, 1732-1745.	0.2	7
46	Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17249-17254.	1.5	6
47	Nonaffine Displacements Encode Collective Conformational Fluctuations in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2508-2516.	2.3	6
48	Spontaneous transmembrane pore formation by short-chain synthetic peptide. <i>Biophysical Journal</i> , 2021, 120, 4557-4574.	0.2	6
49	Hi-C embedded polymer model of <i>Escherichia coli</i> reveals the origin of heterogeneous subdiffusion in chromosomal loci. <i>Physical Review E</i> , 2022, 105, .	0.8	6
50	Mechanism of Coordinated Gating and Signal Transduction in Purine Biosynthetic Enzyme Formylglycinamide Synthetase. <i>ACS Catalysis</i> , 2022, 12, 1930-1944.	5.5	5
51	Sequence-Dependent pK_a Shift Induced by Molecular Self-Assembly: Insights from Computer Simulation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 491-495.	1.2	4
52	Role of β and β^2 relaxations in collapsing dynamics of a polymer chain in supercooled glass-forming liquid. <i>Journal of Chemical Physics</i> , 2019, 150, 114503.	1.2	4
53	Conformational Reorganization of Apolipoprotein E Triggered by Phospholipid Assembly. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5285-5295.	1.2	4
54	Zwitterionic Osmolytes Revive Surface Charges under Salt Stress via Dual Mechanisms. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5660-5668.	2.1	4

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55	Elucidating the Mechanism of Nitrogen Doping in Graphene Oxide: Structural Evolution of Dopants and the Role of Oxygen. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22547-22553.	1.5	3
56	Molecular dynamics simulations elucidate oligosaccharide recognition pathways by galectin-3 at atomic resolution. <i>Journal of Biological Chemistry</i> , 2021, 297, 101271.	1.6	3
57	Role of molecular dynamics in optimising ligand discovery: Case study with novel inhibitor search for peptidyl t-RNA hydrolase. <i>Chemical Physics Impact</i> , 2021, 3, 100048.	1.7	3
58	Impact of Inert Crowders on Host-Guest Recognition Process. <i>Journal of Physical Chemistry B</i> , 0, , .	1.2	3
59	Solvent's Role in Cavity-Ligand Recognition Would Depend on the Mode of Ligand Diffusion. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2952-2958.	1.2	1