Jeetain Mittal

List of Publications by Year
in descending order

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124 papers	13,724 citations	34105 52 h-index	26613 107 g-index
139 all docs	139 docs citations	139 times ranked	12775 citing authors

#	Article	IF	Citations
1	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone Ï•, Ï^ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	5.3	3,696
2	ALS Mutations Disrupt Phase Separation Mediated by Î±-Helical Structure in the TDP-43 Low-Complexity C-Terminal Domain. Structure, 2016, 24, 1537-1549.	3.3	617
3	Balanced Proteinâ€“Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association. Journal of Chemical Theory and Computation, 2014, 10, 5113-5124.	5.3	564
4	Phosphorylation of the <scp>FUS</scp> lowâ€complexity domain disrupts phase separation, aggregation, and toxicity. EMBO Journal, 2017, 36, 2951-2967.	7.8	544
5	Molecular interactions underlying liquidâ^'liquid phase separation of the FUS low-complexity domain. Nature Structural and Molecular Biology, 2019, 26, 637-648.	8.2	463
6	Sequence determinants of protein phase behavior from a coarse-grained model. PLoS Computational Biology, 2018, 14, e1005941.	3.2	427
7	Biomolecular Phase Separation: From Molecular Driving Forces to Macroscopic Properties. Annual Review of Physical Chemistry, 2020, 71, 53-75.	10.8	368
8	Mechanistic View of hnRNPA2 Low-Complexity Domain Structure, Interactions, and Phase Separation Altered by Mutation and Arginine Methylation. Molecular Cell, 2018, 69, 465-479.e7.	9.7	312
9	Relation between single-molecule properties and phase behavior of intrinsically disordered proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9929-9934.	7.1	283
10	TDP-43 Î±-helical structure tunes liquidâ€“liquid phase separation and function. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 5883-5894.	7.1	258
11	Protein Simulations with an Optimized Water Model: Cooperative Helix Formation and Temperature-Induced Unfolded State Collapse. Journal of Physical Chemistry B, 2010, 114, 14916-14923.	2.6	233
12	Identifying sequence perturbations to an intrinsically disordered protein that determine its phase-separation behavior. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 11421-11431.	7.1	202
13	Temperature-Controlled Liquidâ€“Liquid Phase Separation of Disordered Proteins. ACS Central Science, 2019, 5, 821-830.	11.3	199
14	Layering and Position-Dependent Diffusive Dynamics of Confined Fluids. Physical Review Letters, 2008, 100, 145901.	7.8	161
15	Temperature-dependent solvation modulates the dimensions of disordered proteins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5213-5218.	7.1	161
16	A carbon nanotube reporter of microRNA hybridization events in vivo. Nature Biomedical Engineering, 2017, 1, .	22.5	160
17	Excess-entropy-based anomalies for a waterlike fluid. Journal of Chemical Physics, 2006, 125, 244502.	3.0	148
18	Thermodynamics and kinetics of protein folding under confinement. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20233-20238.	7.1	146

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19	Thermodynamics Predicts How Confinement Modifies the Dynamics of the Equilibrium Hard-Sphere Fluid. Physical Review Letters, 2006, 96, 177804.	7.8	133
20	Static and dynamic correlations in water at hydrophobic interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20130-20135.	7.1	132
21	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of Î±-Helix and Î²-Hairpin Formation. Biophysical Journal, 2012, 103, 1045-1051.	0.5	130
22	Molecular Details of Protein Condensates Probed by Microsecond Long Atomistic Simulations. Journal of Physical Chemistry B, 2020, 124, 11671-11679.	2.6	127
23	Molecular-Basis of Single-Walled Carbon Nanotube Recognition by Single-Stranded DNA. Nano Letters, 2012, 12, 1464-1469.	9.1	115
24	Freeâ€energy landscape of the GB1 hairpin in allâ€atom explicit solvent simulations with different force fields: Similarities and differences. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1318-1328.	2.6	112
25	Tackling Force-Field Bias in Protein Folding Simulations: Folding of Villin HP35 and Pin WW Domains in Explicit Water. Biophysical Journal, 2010, 99, L26-L28.	0.5	105
26	Physics-based computational and theoretical approaches to intrinsically disordered proteins. Current Opinion in Structural Biology, 2021, 67, 219-225.	5.7	101
27	Residue-Specific Î±-Helix Propensities from Molecular Simulation. Biophysical Journal, 2012, 102, 1462-1467.	0.5	97
28	Balance between Î± and Î² Structures in Ab Initio Protein Folding. Journal of Physical Chemistry B, 2010, 114, 8790-8798.	2.6	96
29	Quantitative Link between Single-Particle Dynamics and Static Structure of Supercooled Liquids. Journal of Physical Chemistry B, 2006, 110, 18147-18150.	2.6	95
30	Relationships between Self-Diffusivity, Packing Fraction, and Excess Entropy in Simple Bulk and Confined Fluids. Journal of Physical Chemistry B, 2007, 111, 10054-10063.	2.6	94
31	Water Transport through Nanotubes with Varying Interaction Strength between Tube Wall and Water. Journal of Physical Chemistry Letters, 2011, 2, 2978-2983.	4.6	90
32	Simulation methods for liquidâ€“liquid phase separation of disordered proteins. Current Opinion in Chemical Engineering, 2019, 23, 92-98.	7.8	89
33	Improved coarseâ€grained model for studying sequence dependent phase separation of disordered proteins. Protein Science, 2021, 30, 1371-1379.	7.6	85
34	A Carbon Nanotube Optical Reporter Maps Endolysosomal Lipid Flux. ACS Nano, 2017, 11, 10689-10703.	14.6	84
35	Inferring properties of disordered chains from FRET transfer efficiencies. Journal of Chemical Physics, 2018, 148, 123329.	3.0	84
36	Sequence dependent phase separation of protein-polynucleotide mixtures elucidated using molecular simulations. Nucleic Acids Research, 2020, 48, 12593-12603.	14.5	83

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37	Dependence of Protein Folding Stability and Dynamics on the Density and Composition of Macromolecular Crowders. Biophysical Journal, 2010, 98, 315-320.	0.5	81
38	An optical nanoreporter of endolysosomal lipid accumulation reveals enduring effects of diet on hepatic macrophages in vivo. Science Translational Medicine, 2018, 10, .	12.4	80
39	Surface force measurements and simulations of mussel-derived peptide adhesives on wet organic surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 4332-4337.	7.1	77
40	Sequence-Specific Self-Stitching Motif of Short Single-Stranded DNA on a Single-Walled Carbon Nanotube. Journal of the American Chemical Society, 2011, 133, 13545-13550.	13.7	76
41	Crowding Induced Entropy-Enthalpy Compensation in Protein Association Equilibria. Physical Review Letters, 2013, 110, 208102.	7.8	76
42	Interfacial thermodynamics of confined water near molecularly rough surfaces. Faraday Discussions, 2010, 146, 341.	3.2	75
43	Molecular interactions contributing to FUS SYGQ LC-RGG phase separation and co-partitioning with RNA polymerase II heptads. Nature Structural and Molecular Biology, 2021, 28, 923-935.	8.2	75
44	Structural Ensemble of an Intrinsically Disordered Polypeptide. Journal of Physical Chemistry B, 2013, 117, 118-124.	2.6	72
45	Sequence- and Temperature-Dependent Properties of Unfolded and Disordered Proteins from Atomistic Simulations. Journal of Physical Chemistry B, 2015, 119, 14622-14630.	2.6	70
46	Hydropathy Patterning Complements Charge Patterning to Describe Conformational Preferences of Disordered Proteins. Journal of Physical Chemistry Letters, 2020, 11, 3408-3415.	4.6	70
47	Free Energy Surface of an Intrinsically Disordered Protein: Comparison between Temperature Replica Exchange Molecular Dynamics and Bias-Exchange Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 2776-2782.	5.3	69
48	Macromolecular crowding effects on proteinâ€“protein binding affinity and specificity. Journal of Chemical Physics, 2010, 133, 205101.	3.0	68
49	The living interface between synthetic biology and biomaterial design. Nature Materials, 2022, 21, 390-397.	27.5	68
50	Microscopic events in Î²-hairpin folding from alternative unfolded ensembles. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 11087-11092.	7.1	67
51	Instability of Thin Liquid Films by Density Variations: A New Mechanism that Mimics Spinodal Dewetting. Physical Review Letters, 2002, 89, 186101.	7.8	66
52	Does confining the hard-sphere fluid between hard walls change its average properties?. Journal of Chemical Physics, 2007, 126, 244708.	3.0	65
53	Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties. Journal of Physical Chemistry Letters, 2019, 10, 2227-2234.	4.6	65
54	Modest Proteinâ^'Crowder Attractive Interactions Can Counteract Enhancement of Protein Association by Intermolecular Excluded Volume Interactions. Journal of Physical Chemistry B, 2011, 115, 2683-2689.	2.6	62

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55	A predictive coarse-grained model for position-specific effects of post-translational modifications. Biophysical Journal, 2021, 120, 1187-1197.	0.5	56
56	Interaction of Single-Stranded DNA with Curved Carbon Nanotube Is Much Stronger Than with Flat Graphite. Journal of the American Chemical Society, 2014, 136, 12947-12957.	13.7	54
57	Protein Composition Determines the Effect of Crowding on the Properties of Disordered Proteins. Biophysical Journal, 2016, 111, 28-37.	0.5	48
58	Biomolecular Condensates: Sequence Determinants of Phase Separation, Microstructural Organization, Enzymatic Activity, and Material Properties. Journal of Physical Chemistry B, 2021, 125, 3441-3451.	2.6	48
59	Structural Characteristics of Oligomeric DNA Strands Adsorbed onto Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2013, 117, 132-140.	2.6	47
60	Binding between DNA and Carbon Nanotubes Strongly Depends upon Sequence and Chirality. Langmuir, 2014, 30, 3176-3183.	3.5	47
61	Looking at the Disordered Proteins through the Computational Microscope. ACS Central Science, 2018, 4, 534-542.	11.3	46
62	Tyrosine phosphorylation regulates hnRNPA2 granule protein partitioning and reduces neurodegeneration. EMBO Journal, 2021, 40, e105001.	7.8	44
63	Available states and available space: static properties that predict self-diffusivity of confined fluids. Journal of Statistical Mechanics: Theory and Experiment, 2009, 2009, P04006.	2.3	43
64	Molecular Simulations Indicate Marked Differences in the Structure of Amylin Mutants, Correlated with Known Aggregation Propensity. Journal of Physical Chemistry B, 2013, 117, 16066-16075.	2.6	43
65	Refining All-Atom Protein Force Fields for Polar-Rich, Prion-like, Low-Complexity Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2020, 124, 9505-9512.	2.6	40
66	Principles Governing the Phase Separation of Multidomain Proteins. Biochemistry, 2022, 61, 2443-2455.	2.5	40
67	Amphiphilic proteins coassemble into multiphasic condensates and act as biomolecular surfactants. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	37
68	Water transport through functionalized nanotubes with tunable hydrophobicity. Journal of Chemical Physics, 2014, 141, 18C532.	3.0	36
69	Instability and Dewetting of Thin Films Induced by Density Variations. Langmuir, 2002, 18, 10213-10220.	3.5	35
70	Folding Kinetics and Unfolded State Dynamics of the GB1 Hairpin from Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 1743-1753.	5.3	35
71	Biophysical studies of phase separation integrating experimental and computational methods. Current Opinion in Structural Biology, 2021, 70, 78-86.	5.7	35
72	Proteinâ€“protein interactions in a crowded environment. Biophysical Reviews, 2013, 5, 99-108.	3.2	34

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73	Confinement, entropy, and single-particle dynamics of equilibrium hard-sphere mixtures. Journal of Chemical Physics, 2007, 127, 154513.	3.0	32
74	Disorder in Cholesterol-Binding Functionality of CRAC Peptides: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 13169-13174.	2.6	31
75	Lysines in the RNA Polymerase II C-Terminal Domain Contribute to TAF15 Fibril Recruitment. Biochemistry, 2018, 57, 2549-2563.	2.5	31
76	Modest Influence of FRET Chromophores on the Properties of Unfolded Proteins. Biophysical Journal, 2014, 107, 1654-1660.	0.5	29
77	Reversible Kinetic Trapping of FUS Biomolecular Condensates. Advanced Science, 2022, 9, e2104247.	11.2	28
78	Using a sequence-specific coarse-grained model for studying protein liquidâ€“liquid phase separation. Methods in Enzymology, 2021, 646, 1-17.	1.0	27
79	Nâ€terminal acetylation modestly enhances phase separation and reduces aggregation of the lowâ€complexity domain of RNAâ€binding protein fused in sarcoma. Protein Science, 2021, 30, 1337-1349.	7.6	27
80	DNA Base Dimers Are Stabilized by Hydrogen-Bonding Interactions Including Non-Watsonâ€“Crick Pairing Near Graphite Surfaces. Journal of Physical Chemistry B, 2012, 116, 12088-12094.	2.6	26
81	Interplay Between Membrane Composition and Structural Stability of Membrane-Bound hIAPP. Journal of Physical Chemistry B, 2017, 121, 8661-8668.	2.6	25
82	Insights into DNA-mediated interparticle interactions from a coarse-grained model. Journal of Chemical Physics, 2014, 141, 184901.	3.0	23
83	Computational study of trimer self-assembly and fluid phase behavior. Journal of Chemical Physics, 2015, 142, 164901.	3.0	23
84	A hybrid, bottom-up, structurally accurate, GoÂ¯-like coarse-grained protein model. Journal of Chemical Physics, 2019, 151, 044111.	3.0	23
85	Self-assembly of trimer colloids: effect of shape and interaction range. Soft Matter, 2016, 12, 4170-4179.	2.7	22
86	Binary Superlattice Design by Controlling DNA-Mediated Interactions. Langmuir, 2018, 34, 991-998.	3.5	22
87	Smoothing of the GB1 Hairpin Folding Landscape by Interfacial Confinement. Biophysical Journal, 2012, 103, 596-600.	0.5	21
88	Ab Initio Crystallization of Alkanes: Structure and Kinetics of Nuclei Formation. Macromolecules, 2013, 46, 9151-9157.	4.8	21
89	Folding thermodynamics of Î²â€hairpins studied by replicaâ€exchange molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1307-1315.	2.6	21
90	Diffusive Dynamics of Contact Formation in Disordered Polypeptides. Physical Review Letters, 2016, 116, 068102.	7.8	21

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91	Computational modeling highlights the role of the disordered Formin Homology 1 domain in profilinâ€actin transfer. FEBS Letters, 2018, 592, 1804-1816.	2.8	21
92	Using Energy Landscapes To Predict the Properties of Thin Filmsâ€. Journal of Physical Chemistry B, 2004, 108, 19769-19779.	2.6	20
93	To What Extent Does Surface Hydrophobicity Dictate Peptide Folding and Stability near Surfaces?. Langmuir, 2015, 31, 12223-12230.	3.5	20
94	Pair diffusion, hydrodynamic interactions, and available volume in dense fluids. Journal of Chemical Physics, 2012, 137, 034110.	3.0	19
95	Macromolecular Crowding Effects on Coupled Folding and Binding. Journal of Physical Chemistry B, 2014, 118, 12621-12629.	2.6	19
96	Effect of O-Linked Glycosylation on the Equilibrium Structural Ensemble of Intrinsically Disordered Polypeptides. Journal of Physical Chemistry B, 2015, 119, 15583-15592.	2.6	19
97	Assembly of multi-flavored two-dimensional colloidal crystals. Soft Matter, 2017, 13, 5397-5408.	2.7	19
98	Effect of Phosphorylation and O-GlcNAcylation on Proline-Rich Domains of Tau. Journal of Physical Chemistry B, 2020, 124, 1909-1918.	2.6	18
99	Role of solvation in pressure-induced helix stabilization. Journal of Chemical Physics, 2014, 141, 22D522.	3.0	16
100	Grand canonical inverse design of multicomponent colloidal crystals. Soft Matter, 2020, 16, 3187-3194.	2.7	16
101	Deep learning for characterizing the self-assembly of three-dimensional colloidal systems. Soft Matter, 2021, 17, 989-999.	2.7	16
102	Assembly of three-dimensional binary superlattices from multi-flavored particles. Soft Matter, 2018, 14, 6303-6312.	2.7	15
103	Electrostatic Screening Modulates Analyte Binding and Emission of Carbon Nanotubes. Journal of Physical Chemistry C, 2018, 122, 10592-10599.	3.1	14
104	Using symmetry to elucidate the importance of stoichiometry in colloidal crystal assembly. Nature Communications, 2019, 10, 2028.	12.8	14
105	Using Compressibility Factor as a Predictor of Confined Hard-Sphere Fluid Dynamics. Journal of Physical Chemistry B, 2009, 113, 13800-13804.	2.6	13
106	Structural Stability and Binding Strength of a Designed Peptideâ€“Carbon Nanotube Hybrid. Journal of Physical Chemistry C, 2013, 117, 26255-26261.	3.1	13
107	Size-dependent thermodynamic structural selection in colloidal crystallization. Science Advances, 2019, 5, eaaw5912.	10.3	11
108	Alteration of Microstructure in Biopolymeric Hydrogels via Compositional Modification of Resilin-Like Polypeptides. ACS Biomaterials Science and Engineering, 2021, 7, 4244-4257.	5.2	11

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109	Equilibrium and nonequilibrium dynamics of soft sphere fluids. Soft Matter, 2015, 11, 5274-5281.	2.7	10
110	Designing molecular building blocks for the self-assembly of complex porous networks. Molecular Systems Design and Engineering, 2019, 4, 644-653.	3.4	10
111	Effect of Nonionic Surfactant on Association/Dissociation Transition of DNA-Functionalized Colloids. Langmuir, 2016, 32, 10017-10025.	3.5	7
112	Modelling and simulation of DNA-mediated self-assembly for superlattice design. Molecular Simulation, 2019, 45, 1203-1210.	2.0	7
113	Temperature-Controlled Reconfigurable Nanoparticle Binary Superlattices. ACS Nano, 2021, 15, 8466-8473.	14.6	7
114	Extension of the Einstein molecule method for solid free energy calculation to non-periodic and semi-periodic systems. Journal of Chemical Physics, 2019, 151, 054105.	3.0	6
115	Self-Assembly of DNA-Functionalized Nanoparticles Guided by Binding Kinetics. Journal of Physical Chemistry B, 2020, 124, 11593-11599.	2.6	5
116	Symmetry-Based Crystal Structure Enumeration in Two Dimensions. Journal of Physical Chemistry A, 2020, 124, 3276-3285.	2.5	4
117	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. Journal of Physical Chemistry C, 2020, 124, 16350-16361.	3.1	4
118	Living cells as test tubes. Nature Chemical Biology, 2020, 16, 934-935.	8.0	3
119	Effect of molecular structure on fluid transport through carbon nanotubes. Molecular Physics, 2014, 112, 2658-2664.	1.7	1
120	Coarse-Grained Simulations of Intrinsically Disordered Proteins in the Context of Liquid-Liquid Phase Separation. Biophysical Journal, 2018, 114, 431a-432a.	0.5	1
121	A High-Throughput Approach to Phase Separation of Disordered Proteins. Biophysical Journal, 2019, 116, 350a.	0.5	1
122	Multiscale Model of the Formin Homology 1 Domain Illustrates its Role in Regulation of Actin Polymerization. Biophysical Journal, 2018, 114, 144a.	0.5	0
123	Identifying Sequence-Determinants of Protein Liquid-Liquid Phase Separation. Biophysical Journal, 2019, 116, 4a.	0.5	0
124	Impact of Hydrophobic Patterning on Conformational Ensemble of Disordered Proteins. Biophysical Journal, 2020, 118, 214a.	0.5	0