Jeetain Mittal

List of Publications by Citations

126 papers	9,130 citations	47 h-index	94 g-index
139 ext. papers	11,610 ext. citations	6.3 avg, IF	6.74 L-index

#	Paper	IF	Citations
126	Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone φ, ψ and side-chain χ1 and χ2 dihedral angles. *Journal of Chemical Theory and Computation*, **2012**, 8, 3257-3273	6.4	2511
125	ALS Mutations Disrupt Phase Separation Mediated by α-Helical Structure in the TDP-43 Low-Complexity C-Terminal Domain. *Structure*, **2016**, 24, 1537-49	5.2	409
124	Balanced Protein-Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association. *Journal of Chemical Theory and Computation*, **2014**, 10, 5113-5124	6.4	409
123	Phosphorylation of the FUS low-complexity domain disrupts phase separation, aggregation, and toxicity. *EMBO Journal*, **2017**, 36, 2951-2967	13	365
122	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	17.6	215
121	Molecular interactions underlying liquid-liquid phase separation of the FUS low-complexity domain. *Nature Structural and Molecular Biology*, **2019**, 26, 637-648	17.6	211
120	Sequence determinants of protein phase behavior from a coarse-grained model. *PLoS Computational Biology*, **2018**, 14, e1005941	5	209
119	Protein simulations with an optimized water model: cooperative helix formation and temperature-induced unfolded state collapse. *Journal of Physical Chemistry B*, **2010**, 114, 14916-23	3.4	195
118	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	11.5	149
117	Excess-entropy-based anomalies for a waterlike fluid. *Journal of Chemical Physics*, **2006**, 125, 244502	3.9	146
116	Layering and position-dependent diffusive dynamics of confined fluids. *Physical Review Letters*, **2008**, 100, 145901	7.4	144
115	Thermodynamics and kinetics of protein folding under confinement. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 20233-8	11.5	131
114	Temperature-dependent solvation modulates the dimensions of disordered proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 5213-8	11.5	125
113	Static and dynamic correlations in water at hydrophobic interfaces. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 20130-5	11.5	121
112	Thermodynamics predicts how confinement modifies the dynamics of the equilibrium hard-sphere fluid. *Physical Review Letters*, **2006**, 96, 177804	7.4	121
111	TDP-43 α-helical structure tunes liquid-liquid phase separation and function. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 5883-5894	11.5	119
110	Biomolecular Phase Separation: From Molecular Driving Forces to Macroscopic Properties. *Annual Review of Physical Chemistry*, **2020**, 71, 53-75	15.7	116

109	A Carbon Nanotube Reporter of miRNA Hybridization Events In Vivo. *Nature Biomedical Engineering*, **2017**, 1,	19	111
108	Temperature-Controlled Liquid-Liquid Phase Separation of Disordered Proteins. *ACS Central Science*, **2019**, 5, 821-830	16.8	108
107	Inclusion of many-body effects in the additive CHARMM protein CMAP potential results in enhanced cooperativity of α-helix and β-hairpin formation. *Biophysical Journal*, **2012**, 103, 1045-51	2.9	105
106	Free-energy landscape of the GB1 hairpin in all-atom explicit solvent simulations with different force fields: Similarities and differences. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 1318-28	4.2	103
105	Molecular-basis of single-walled carbon nanotube recognition by single-stranded DNA. *Nano Letters*, **2012**, 12, 1464-9	11.5	98
104	Tackling force-field bias in protein folding simulations: folding of Villin HP35 and Pin WW domains in explicit water. *Biophysical Journal*, **2010**, 99, L26-8	2.9	96
103	Quantitative link between single-particle dynamics and static structure of supercooled liquids. *Journal of Physical Chemistry B*, **2006**, 110, 18147-50	3.4	93
102	Relationships between self-diffusivity, packing fraction, and excess entropy in simple bulk and confined fluids. *Journal of Physical Chemistry B*, **2007**, 111, 10054-63	3.4	88
101	Balance between alpha and beta structures in ab initio protein folding. *Journal of Physical Chemistry B*, **2010**, 114, 8790-8	3.4	87
100	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	11.5	81
99	Water Transport through Nanotubes with Varying Interaction Strength between Tube Wall and Water. *Journal of Physical Chemistry Letters*, **2011**, 2, 2978-2983	6.4	81
98	Residue-specific α-helix propensities from molecular simulation. *Biophysical Journal*, **2012**, 102, 1462-7	2.9	72
97	Sequence-specific self-stitching motif of short single-stranded DNA on a single-walled carbon nanotube. *Journal of the American Chemical Society*, **2011**, 133, 13545-50	16.4	71
96	Dependence of protein folding stability and dynamics on the density and composition of macromolecular crowders. *Biophysical Journal*, **2010**, 98, 315-20	2.9	71
95	Interfacial thermodynamics of confined water near molecularly rough surfaces. *Faraday Discussions*, **2010**, 146, 341-52; discussion 367-93, 395-401	3.6	70
94	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, 4332-7	11.5	65
93	Structural ensemble of an intrinsically disordered polypeptide. *Journal of Physical Chemistry B*, **2013**, 117, 118-24	3.4	64
92	Inferring properties of disordered chains from FRET transfer efficiencies. *Journal of Chemical Physics*, **2018**, 148, 123329	3.9	63

91	Microscopic events in hairpin folding from alternative unfolded ensembles. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 11087-92	11.5	62
90	Instability of thin liquid films by density variations: a new mechanism that mimics spinodal dewetting. *Physical Review Letters*, **2002**, 89, 186101	7.4	62
89	Crowding induced entropy-enthalpy compensation in protein association equilibria. *Physical Review Letters*, **2013**, 110, 208102	7.4	61
88	Does confining the hard-sphere fluid between hard walls change its average properties?. *Journal of Chemical Physics*, **2007**, 126, 244708	3.9	61
87	Macromolecular crowding effects on protein-protein binding affinity and specificity. *Journal of Chemical Physics*, **2010**, 133, 205101	3.9	56
86	Modest protein-crowder attractive interactions can counteract enhancement of protein association by intermolecular excluded volume interactions. *Journal of Physical Chemistry B*, **2011**, 115, 2683-9	3.4	55
85	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, 2776-82	6.4	53
84	A Carbon Nanotube Optical Reporter Maps Endolysosomal Lipid Flux. *ACS Nano*, **2017**, 11, 10689-10703	16.7	52
83	Interaction of single-stranded DNA with curved carbon nanotube is much stronger than with flat graphite. *Journal of the American Chemical Society*, **2014**, 136, 12947-57	16.4	50
82	Sequence- and Temperature-Dependent Properties of Unfolded and Disordered Proteins from Atomistic Simulations. *Journal of Physical Chemistry B*, **2015**, 119, 14622-30	3.4	49
81	Simulation methods for liquid-liquid phase separation of disordered proteins. *Current Opinion in Chemical Engineering*, **2019**, 23, 92-98	5.4	47
80	An optical nanoreporter of endolysosomal lipid accumulation reveals enduring effects of diet on hepatic macrophages in vivo. *Science Translational Medicine*, **2018**, 10,	17.5	47
79	Structural characteristics of oligomeric DNA strands adsorbed onto single-walled carbon nanotubes. *Journal of Physical Chemistry B*, **2013**, 117, 132-40	3.4	43
78	Available states and available space: static properties that predict self-diffusivity of confined fluids. *Journal of Statistical Mechanics: Theory and Experiment*, **2009**, 2009, P04006	1.9	41
77	Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties. *Journal of Physical Chemistry Letters*, **2019**, 10, 2227-2234	6.4	39
76	Protein Composition Determines the Effect of Crowding on the Properties of Disordered Proteins. *Biophysical Journal*, **2016**, 111, 28-37	2.9	38
75	Molecular simulations indicate marked differences in the structure of amylin mutants, correlated with known aggregation propensity. *Journal of Physical Chemistry B*, **2013**, 117, 16066-75	3.4	37
74	Binding between DNA and carbon nanotubes strongly depends upon sequence and chirality. *Langmuir*, **2014**, 30, 3176-83	4	36

73	Hydropathy Patterning Complements Charge Patterning to Describe Conformational Preferences of Disordered Proteins. *Journal of Physical Chemistry Letters*, **2020**, 11, 3408-3415	6.4	34
72	Instability and Dewetting of Thin Films Induced by Density Variations. *Langmuir*, **2002**, 18, 10213-10220	4	34
71	Sequence dependent phase separation of protein-polynucleotide mixtures elucidated using molecular simulations. *Nucleic Acids Research*, **2020**, 48, 12593-12603	20.1	34
70	Molecular Details of Protein Condensates Probed by Microsecond Long Atomistic Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 11671-11679	3.4	32
69	Folding Kinetics and Unfolded State Dynamics of the GB1 Hairpin from Molecular Simulation. *Journal of Chemical Theory and Computation*, **2013**, 9, 1743-53	6.4	32
68	Physics-based computational and theoretical approaches to intrinsically disordered proteins. *Current Opinion in Structural Biology*, **2021**, 67, 219-225	8.1	32
67	Water transport through functionalized nanotubes with tunable hydrophobicity. *Journal of Chemical Physics*, **2014**, 141, 18C532	3.9	31
66	Confinement, entropy, and single-particle dynamics of equilibrium hard-sphere mixtures. *Journal of Chemical Physics*, **2007**, 127, 154513	3.9	30
65	Looking at the Disordered Proteins through the Computational Microscope. *ACS Central Science*, **2018**, 4, 534-542	16.8	27
64	A predictive coarse-grained model for position-specific effects of post-translational modifications. *Biophysical Journal*, **2021**, 120, 1187-1197	2.9	27
63	Disorder in cholesterol-binding functionality of CRAC peptides: a molecular dynamics study. *Journal of Physical Chemistry B*, **2014**, 118, 13169-74	3.4	25
62	Modest influence of FRET chromophores on the properties of unfolded proteins. *Biophysical Journal*, **2014**, 107, 1654-60	2.9	25
61	Protein-protein interactions in a crowded environment. *Biophysical Reviews*, **2013**, 5, 99-108	3.7	24
60	Computational study of trimer self-assembly and fluid phase behavior. *Journal of Chemical Physics*, **2015**, 142, 164901	3.9	22
59	Smoothing of the GB1 hairpin folding landscape by interfacial confinement. *Biophysical Journal*, **2012**, 103, 596-600	2.9	21
58	Improved coarse-grained model for studying sequence dependent phase separation of disordered proteins. *Protein Science*, **2021**, 30, 1371-1379	6.3	21
57	Lysines in the RNA Polymerase II C-Terminal Domain Contribute to TAF15 Fibril Recruitment. *Biochemistry*, **2018**, 57, 2549-2563	3.2	20
56	DNA base dimers are stabilized by hydrogen-bonding interactions including non-Watson-Crick pairing near graphite surfaces. *Journal of Physical Chemistry B*, **2012**, 116, 12088-94	3.4	20

55	Using Energy Landscapes To Predict the Properties of Thin Films *Journal of Physical Chemistry B*, **2004**, 108, 19769-19779	3.4	20
54	To What Extent Does Surface Hydrophobicity Dictate Peptide Folding and Stability near Surfaces?. *Langmuir*, **2015**, 31, 12223-30	4	19
53	Diffusive Dynamics of Contact Formation in Disordered Polypeptides. *Physical Review Letters*, **2016**, 116, 068102	7.4	19
52	Interplay Between Membrane Composition and Structural Stability of Membrane-Bound hIAPP. *Journal of Physical Chemistry B*, **2017**, 121, 8661-8668	3.4	18
51	Insights into DNA-mediated interparticle interactions from a coarse-grained model. *Journal of Chemical Physics*, **2014**, 141, 184901	3.9	18
50	Self-assembly of trimer colloids: effect of shape and interaction range. *Soft Matter*, **2016**, 12, 4170-9	3.6	18
49	Binary Superlattice Design by Controlling DNA-Mediated Interactions. *Langmuir*, **2018**, 34, 991-998	4	18
48	Macromolecular crowding effects on coupled folding and binding. *Journal of Physical Chemistry B*, **2014**, 118, 12621-9	3.4	17
47	Folding thermodynamics of hairpins studied by replica-exchange molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1307-15	4.2	17
46	Pair diffusion, hydrodynamic interactions, and available volume in dense fluids. *Journal of Chemical Physics*, **2012**, 137, 034110	3.9	17
45	Effect of O-Linked Glycosylation on the Equilibrium Structural Ensemble of Intrinsically Disordered Polypeptides. *Journal of Physical Chemistry B*, **2015**, 119, 15583-92	3.4	16
44	Ab Initio Crystallization of Alkanes: Structure and Kinetics of Nuclei Formation. *Macromolecules*, **2013**, 46, 9151-9157	5.5	15
43	Role of solvation in pressure-induced helix stabilization. *Journal of Chemical Physics*, **2014**, 141, 22D522	3.9	15
42	Tyrosine phosphorylation regulates hnRNPA2 granule protein partitioning and reduces neurodegeneration. *EMBO Journal*, **2021**, 40, e105001	13	15
41	Assembly of multi-flavored two-dimensional colloidal crystals. *Soft Matter*, **2017**, 13, 5397-5408	3.6	14
40	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	3.4	13
39	A hybrid, bottom-up, structurally accurate, Go-like coarse-grained protein model. *Journal of Chemical Physics*, **2019**, 151, 044111	3.9	12
38	Using compressibility factor as a predictor of confined hard-sphere fluid dynamics. *Journal of Physical Chemistry B*, **2009**, 113, 13800-4	3.4	12

37	Using symmetry to elucidate the importance of stoichiometry in colloidal crystal assembly. *Nature Communications*, **2019**, 10, 2028	17.4	11
36	Assembly of three-dimensional binary superlattices from multi-flavored particles. *Soft Matter*, **2018**, 14, 6303-6312	3.6	11
35	Structural Stability and Binding Strength of a Designed Peptide-Carbon Nanotube Hybrid. *Journal of Physical Chemistry C*, **2013**, 117, 26255-26261	3.8	11
34	Biomolecular Condensates: Sequence Determinants of Phase Separation, Microstructural Organization, Enzymatic Activity, and Material Properties. *Journal of Physical Chemistry B*, **2021**, 125, 3441-3451	3.4	11
33	N-terminal acetylation modestly enhances phase separation and reduces aggregation of the low-complexity domain of RNA-binding protein fused in sarcoma. *Protein Science*, **2021**, 30, 1337-1349	6.3	11
32	Equilibrium and nonequilibrium dynamics of soft sphere fluids. *Soft Matter*, **2015**, 11, 5274-81	3.6	10
31	Grand canonical inverse design of multicomponent colloidal crystals. *Soft Matter*, **2020**, 16, 3187-3194	3.6	10
30	Computational modeling highlights the role of the disordered Formin Homology 1 domain in profilin-actin transfer. *FEBS Letters*, **2018**, 592, 1804-1816	3.8	10
29	Effect of Phosphorylation and O-GlcNAcylation on Proline-Rich Domains of Tau. *Journal of Physical Chemistry B*, **2020**, 124, 1909-1918	3.4	9
28	Electrostatic Screening Modulates Analyte Binding and Emission of Carbon Nanotubes. *Journal of Physical Chemistry C*, **2018**, 122, 10592-10599	3.8	9
27	Size-dependent thermodynamic structural selection in colloidal crystallization. *Science Advances*, **2019**, 5, eaaw5912	14.3	8
26	Designing Molecular Building Blocks for the Self-assembly of Complex Porous Networks. *Molecular Systems Design and Engineering*, **2019**, 4,	4.6	7
25	Effect of Nonionic Surfactant on Association/Dissociation Transition of DNA-Functionalized Colloids. *Langmuir*, **2016**, 32, 10017-10025	4	7
24	Using a sequence-specific coarse-grained model for studying protein liquid-liquid phase separation. *Methods in Enzymology*, **2021**, 646, 1-17	1.7	7
23	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	17.6	6
22	A predictive coarse-grained model for position-specific effects of post-translational modifications on disordered protein phase separation		6
21	Modelling and simulation of DNA-mediated self-assembly for superlattice design. *Molecular Simulation*, **2019**, 45, 1203-1210	2	5
20	Identifying Sequence Perturbations to an Intrinsically Disordered Protein that Determine Its Phase Separation Behavior		5

19	Molecular details of protein condensates probed by microsecond-long atomistic simulations		5
18	TDP-43 α-helical structure tunes liquid-liquid phase separation and function		4
17	Biophysical studies of phase separation integrating experimental and computational methods. *Current Opinion in Structural Biology*, **2021**, 70, 78-86	8.1	4
16	The living interface between synthetic biology and biomaterial design.. *Nature Materials*, **2022**, 21, 390-397	27	4
15	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,	11.5	4
14	Symmetry-Based Crystal Structure Enumeration in Two Dimensions. *Journal of Physical Chemistry A*, **2020**, 124, 3276-3285	2.8	3
13	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	3.9	3
12	Living cells as test tubes. *Nature Chemical Biology*, **2020**, 16, 934-935	11.7	3
11	Temperature-Controlled Reconfigurable Nanoparticle Binary Superlattices. *ACS Nano*, **2021**, 15, 8466-8473	13.7	3
10	Deep learning for characterizing the self-assembly of three-dimensional colloidal systems. *Soft Matter*, **2021**, 17, 989-999	3.6	3
9	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. *Journal of Physical Chemistry C*, **2020**, 124,	3.8	2
8	Hydropathy patterning complements charge patterning to describe conformational preferences of disordered proteins		2
7	Tyrosine phosphorylation regulates hnRNPA2 granule protein partitioning & reduces neurodegeneration		2
6	Sequence dependent co-phase separation of RNA-protein mixtures elucidated using molecular simulations		2
5	Amphiphilic proteins coassemble into multiphasic condensates and act as biomolecular surfactants		2
4	Alteration of Microstructure in Biopolymeric Hydrogels Compositional Modification of Resilin-Like Polypeptides. *ACS Biomaterials Science and Engineering*, **2021**, 7, 4244-4257	5.5	2
3	Self-Assembly of DNA-Functionalized Nanoparticles Guided by Binding Kinetics. *Journal of Physical Chemistry B*, **2020**, 124, 11593-11599	3.4	1
2	Effect of molecular structure on fluid transport through carbon nanotubes. *Molecular Physics*, **2014**, 112, 2658-2664	1.7	1

1	Reversible Kinetic Trapping of FUS Biomolecular Condensates. *Advanced Science*, **2021**, e2104247	13.6	1