

Dave Thirumalai

List of Publications by Year in descending order

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277
papers

23,591
citations

6254

80
h-index

10158

140
g-index

317
all docs

317
docs citations

317
times ranked

11465
citing authors

#	ARTICLE	IF	CITATIONS
1	Navigating the folding routes. <i>Science</i> , 1995, 267, 1619-1620.	12.6	1,111
2	Scaling concepts for the dynamics of viscous liquids near an ideal glassy state. <i>Physical Review A</i> , 1989, 40, 1045-1054.	2.5	878
3	Molecular crowding enhances native state stability and refolding rates of globular proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 4753-4758.	7.1	512
4	Urea denaturation by stronger dispersion interactions with proteins than water implies a 2-stage unfolding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 16928-16933.	7.1	470
5	p-spin-interaction spin-glass models: Connections with the structural glass problem. <i>Physical Review B</i> , 1987, 36, 5388-5397.	3.2	457
6	Protein folding kinetics: timescales, pathways and energy landscapes in terms of sequence-dependent properties. <i>Folding & Design</i> , 1997, 2, 1-22.	4.5	390
7	Chaperonin-Mediated Protein Folding. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 2001, 30, 245-269.	18.3	364
8	Dissecting the Assembly of A β Amyloid Peptides into Antiparallel β Sheets. <i>Structure</i> , 2003, 11, 295-307.	3.3	360
9	The nature of folded states of globular proteins. <i>Biopolymers</i> , 1992, 32, 695-709.	2.4	356
10	Kinetics and thermodynamics of folding in model proteins.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1993, 90, 6369-6372.	7.1	345
11	Monomer adds to preformed structured oligomers of A β -peptides by a two-stage dock-lock mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 111-116.	7.1	344
12	Kinetics of protein folding: Nucleation mechanism, time scales, and pathways. <i>Biopolymers</i> , 1995, 36, 83-102.	2.4	340
13	Dynamics of the Structural Glass Transition and the p-Spin Interaction Spin-Glass Model. <i>Physical Review Letters</i> , 1987, 58, 2091-2094.	7.8	325
14	Interactions between Hydrophobic and Ionic Solutes in Aqueous Guanidinium Chloride and Urea Solutions: A Lessons for Protein Denaturation Mechanism. <i>Journal of the American Chemical Society</i> , 2007, 129, 7346-7353.	13.7	324
15	Pair potentials for protein folding: Choice of reference states and sensitivity of predicted native states to variations in the interaction schemes. <i>Protein Science</i> , 1999, 8, 361-369.	7.6	302
16	Role of Water in Protein Aggregation and Amyloid Polymorphism. <i>Accounts of Chemical Research</i> , 2012, 45, 83-92.	15.6	301
17	Hydrophobic Interactions in Aqueous Urea Solutions with Implications for the Mechanism of Protein Denaturation. <i>Journal of the American Chemical Society</i> , 1998, 120, 427-428.	13.7	290
18	Kinetics of Folding of Proteins and RNA. <i>Accounts of Chemical Research</i> , 1996, 29, 433-439.	15.6	256

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19	RNA and Protein Folding: Common Themes and Variations. <i>Biochemistry</i> , 2005, 44, 4957-4970.	2.5	252
20	Toward a Molecular Theory of Early and Late Events in Monomer to Amyloid Fibril Formation. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 437-463.	10.8	249
21	Low-frequency normal modes that describe allosteric transitions in biological nanomachines are robust to sequence variations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 7664-7669.	7.1	248
22	Mechanisms and kinetics of beta -hairpin formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2000, 97, 2544-2549.	7.1	244
23	Chaperonin-facilitated protein folding: optimization of rate and yield by an iterative annealing mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1996, 93, 4030-4035.	7.1	242
24	Viscosity Dependence of the Folding Rates of Proteins. <i>Physical Review Letters</i> , 1997, 79, 317-320.	7.8	230
25	Capturing the essence of folding and functions of biomolecules using coarse-grained models. <i>Nature Communications</i> , 2011, 2, 487.	12.8	222
26	Mechanical unfolding of RNA hairpins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6789-6794.	7.1	215
27	Pathways and Kinetic Barriers in Mechanical Unfolding and Refolding of RNA and Proteins. <i>Structure</i> , 2006, 14, 1633-1645.	3.3	201
28	Dynamics of Asp23~Lys28 Salt-Bridge Formation in A ¹² 10-35 Monomers. <i>Journal of the American Chemical Society</i> , 2006, 128, 16159-16168.	13.7	200
29	EARLY EVENTS IN RNA FOLDING. <i>Annual Review of Physical Chemistry</i> , 2001, 52, 751-762.	10.8	195
30	Folding of RNA involves parallel pathways. <i>Journal of Molecular Biology</i> , 1997, 273, 7-13.	4.2	192
31	Theoretical Perspectives on Protein Folding. <i>Annual Review of Biophysics</i> , 2010, 39, 159-183.	10.0	183
32	Effects of denaturants and osmolytes on proteins are accurately predicted by the molecular transfer model. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 13403-13408.	7.1	182
33	Path integral Monte Carlo studies of the behavior of excess electrons in simple fluids. <i>Journal of Chemical Physics</i> , 1987, 86, 5689-5702.	3.0	179
34	Role of counterion condensation in folding of the Tetrahymena ribozyme. I. Equilibrium stabilization by cations. <i>Journal of Molecular Biology</i> , 2001, 306, 1157-1166.	4.2	179
35	From Minimal Models to Real Proteins: Time Scales for Protein Folding Kinetics. <i>Journal De Physique, I</i> , 1995, 5, 1457-1467.	1.2	178
36	Charge Density of Divalent Metal Cations Determines RNA Stability. <i>Journal of the American Chemical Society</i> , 2007, 129, 2676-2682.	13.7	169

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37	Native topology determines force-induced unfolding pathways in globular proteins. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 7254-7259.	7.1	164
38	Deciphering the timescales and mechanisms of protein folding using minimal off-lattice models. Current Opinion in Structural Biology, 1999, 9, 197-207.	5.7	163
39	Ergodic behavior in supercooled liquids and in glasses. Physical Review A, 1989, 39, 3563-3574.	2.5	161
40	Exploring protein aggregation and self-propagation using lattice models: Phase diagram and kinetics. Protein Science, 2002, 11, 1036-1049.	7.6	160
41	Asymmetry in the Shapes of Folded and Denatured States of Proteins. Journal of Physical Chemistry B, 2004, 108, 6564-6570.	2.6	158
42	Kinetics and Thermodynamics of Folding of a de Novo Designed Four-helix Bundle Protein. Journal of Molecular Biology, 1996, 263, 323-343.	4.2	150
43	Can energy landscape roughness of proteins and RNA be measured by using mechanical unfolding experiments?. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 10249-10253.	7.1	148
44	Influence of Preformed Asp23~Lys28 Salt Bridge on the Conformational Fluctuations of Monomers and Dimers of A1 ² Peptides with Implications for Rates of Fibril Formation. Journal of Physical Chemistry B, 2009, 113, 1162-1172.	2.6	147
45	Revealing the bifurcation in the unfolding pathways of GFP by using single-molecule experiments and simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20268-20273.	7.1	145
46	Ribosome exit tunnel can entropically stabilize \hat{A} -helices. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 18956-18961.	7.1	140
47	Coarse-Grained Model for Predicting RNA Folding Thermodynamics. Journal of Physical Chemistry B, 2013, 117, 4901-4911.	2.6	140
48	Dynamics of allosteric transitions in GroEL. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18939-18944.	7.1	139
49	Activated dynamics, loss of ergodicity, and transport in supercooled liquids. Physical Review E, 1993, 47, 479-489.	2.1	134
50	Exploring the kinetic requirements for enhancement of protein folding rates in the GroEL cavity. Journal of Molecular Biology, 1999, 287, 627-644.	4.2	134
51	Random solutions from a regular density functional Hamiltonian: a static and dynamical theory for the structural glass transition. Journal of Physics A, 1989, 22, L149-L155.	1.6	133
52	Minimum energy compact structures of random sequences of heteropolymers. Physical Review Letters, 1993, 71, 2505-2508.	7.8	133
53	Cooperativity in protein folding: from lattice models with sidechains to real proteins. Folding & Design, 1998, 3, 127-139.	4.5	129
54	Interphase human chromosome exhibits out of equilibrium glassy dynamics. Nature Communications, 2018, 9, 3161.	12.8	127

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55	Collapse transition in proteins. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 83-93.	2.8	125
56	Sequence Effects on Size, Shape, and Structural Heterogeneity in Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3462-3474.	2.6	125
57	Network of Dynamically Important Residues in the Open/Closed Transition in Polymerases Is Strongly Conserved. <i>Structure</i> , 2005, 13, 565-577.	3.3	117
58	Size, shape, and flexibility of RNA structures. <i>Journal of Chemical Physics</i> , 2006, 125, 194905.	3.0	117
59	<i>Colloquium</i>: Random first order transition theory concepts in biology and physics. <i>Reviews of Modern Physics</i> , 2015, 87, 183-209.	45.6	117
60	Role of counterion condensation in folding of the Tetrahymena ribozyme II. Counterion-dependence of folding kinetics. <i>Journal of Molecular Biology</i> , 2001, 309, 57-68.	4.2	114
61	Allosteric Transitions in the Chaperonin GroEL are Captured by a Dominant Normal Mode that is Most Robust to Sequence Variations. <i>Biophysical Journal</i> , 2007, 93, 2289-2299.	0.5	111
62	How do metal ions direct ribozyme folding?. <i>Nature Chemistry</i> , 2015, 7, 793-801.	13.6	110
63	Effects of Macromolecular Crowding on the Collapse of Biopolymers. <i>Physical Review Letters</i> , 2015, 114, 068303.	7.8	109
64	Comparison between dynamical theories and metastable states in regular and glassy mean-field spin models with underlying first-order-like phase transitions. <i>Physical Review A</i> , 1988, 37, 4439-4448.	2.5	106
65	Protein folding guides disulfide bond formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 11241-11246.	7.1	105
66	Factors Governing Fibrillogenesis of Polypeptide Chains Revealed by Lattice Models. <i>Physical Review Letters</i> , 2010, 105, 218101.	7.8	104
67	Mean-field soft-spin Potts glass model: Statics and dynamics. <i>Physical Review B</i> , 1988, 37, 5342-5350.	3.2	103
68	Synergy between intrinsically disordered domains and structured proteins amplifies membrane curvature sensing. <i>Nature Communications</i> , 2018, 9, 4152.	12.8	102
69	Stretching single-domain proteins: Phase diagram and kinetics of force-induced unfolding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1999, 96, 6166-6170.	7.1	101
70	Assembly mechanisms of RNA pseudoknots are determined by the stabilities of constituent secondary structures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 17349-17354.	7.1	100
71	Time scales and pathways for kinetic energy relaxation in solvated proteins: Application to carbonmonoxy myoglobin. <i>Journal of Chemical Physics</i> , 2000, 113, 7702-7711.	3.0	99
72	Theoretical predictions of folding pathways by using the proximity rule, with applications to bovine pancreatic trypsin inhibitor.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1995, 92, 1277-1281.	7.1	97

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73	Lattice models for proteins reveal multiple folding nuclei for nucleation-collapse mechanism 1 Edited by A. R. Fersht. <i>Journal of Molecular Biology</i> , 1998, 282, 471-492.	4.2	96
74	Structures of Î² ² -Amyloid Peptide 1âˆ40, 1âˆ42, and 1âˆ55â€”the 672âˆ726 Fragment of APPâ€”in a Membrane Environment with Implications for Interactions with Î²-Secretase. <i>Journal of the American Chemical Society</i> , 2009, 131, 17843-17852.	13.7	95
75	Electrostatic Persistence Length of a Polyelectrolyte Chain. <i>Macromolecules</i> , 1995, 28, 577-581.	4.8	91
76	Magnesium-dependent folding of self-splicing RNA: Exploring the link between cooperativity, thermodynamics, and kinetics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1999, 96, 6149-6154.	7.1	91
77	Forced-Unfolding and Force-Quench Refolding of RNA Hairpins. <i>Biophysical Journal</i> , 2006, 90, 3410-3427.	0.5	91
78	Thermal denaturation and folding rates of single domain proteins: size matters. <i>Polymer</i> , 2004, 45, 573-579.	3.8	89
79	How accurate are polymer models in the analysis of FÃ¶rster resonance energy transfer experiments on proteins?. <i>Journal of Chemical Physics</i> , 2009, 130, 124903.	3.0	89
80	Kinetic partitioning mechanism as a unifying theme in the folding of biomolecules. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 14-22.	1.4	87
81	Metal Ion Dependence of Cooperative Collapse Transitions in RNA. <i>Journal of Molecular Biology</i> , 2009, 393, 753-764.	4.2	86
82	Crowding Promotes the Switch from Hairpin to Pseudoknot Conformation in Human Telomerase RNA. <i>Journal of the American Chemical Society</i> , 2011, 133, 11858-11861.	13.7	86
83	Nanoporeâ€”Protein Interactions Dramatically Alter Stability and Yield of the Native State in Restricted Spaces. <i>Journal of Molecular Biology</i> , 2006, 357, 632-643.	4.2	85
84	Collapse kinetics and chevron plots from simulations of denaturant-dependent folding of globular proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 7787-7792.	7.1	85
85	Hidden complexity in the isomerization dynamics of Holliday junctions. <i>Nature Chemistry</i> , 2012, 4, 907-914.	13.6	85
86	Effects of pH on Proteins: Predictions for Ensemble and Single-Molecule Pulling Experiments. <i>Journal of the American Chemical Society</i> , 2012, 134, 979-987.	13.7	85
87	Determination of network of residues that regulate allostery in protein families using sequence analysis. <i>Protein Science</i> , 2006, 15, 258-268.	7.6	84
88	Multiple protein folding nuclei and the transition state ensemble in two-state proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 43, 465-475.	2.6	83
89	Measuring the energy landscape roughness and the transition state location of biomolecules using single molecule mechanical unfolding experiments. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 113101.	1.8	83
90	Mechanical Unfolding of RNA: From Hairpins to Structures with Internal Multiloops. <i>Biophysical Journal</i> , 2007, 92, 731-743.	0.5	83

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91	Dry amyloid fibril assembly in a yeast prion peptide is mediated by long-lived structures containing water wires. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 21459-21464.	7.1	82
92	Symmetry, Rigidity, and Allosteric Signaling: From Monomeric Proteins to Molecular Machines. <i>Chemical Reviews</i> , 2019, 119, 6788-6821.	47.7	82
93	Modeling the role of disulfide bonds in protein folding: Entropic barriers and pathways. <i>Proteins: Structure, Function and Bioinformatics</i> , 1995, 22, 27-40.	2.6	80
94	Relative Stability of Helices Determines the Folding Landscape of Adenine Riboswitch Aptamers. <i>Journal of the American Chemical Society</i> , 2008, 130, 14080-14081.	13.7	80
95	From mechanical folding trajectories to intrinsic energy landscapes of biopolymers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 4500-4505.	7.1	80
96	Transmembrane Structures of Amyloid Precursor Protein Dimer Predicted by Replica-Exchange Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2009, 131, 3438-3439.	13.7	79
97	Linking rates of folding in lattice models of proteins with underlying thermodynamic characteristics. <i>Journal of Chemical Physics</i> , 1998, 109, 4119-4125.	3.0	78
98	Static properties of polymer chains in porous media. <i>Journal of Chemical Physics</i> , 1989, 90, 4542-4559.	3.0	77
99	Allosteric Wiring Diagrams in the Transitions that Drive the GroEL Reaction Cycle. <i>Journal of Molecular Biology</i> , 2009, 387, 390-406.	4.2	77
100	Caging helps proteins fold. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 11195-11197.	7.1	75
101	Force-dependent hopping rates of RNA hairpins can be estimated from accurate measurement of the folding landscapes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 9604-9609.	7.1	74
102	Impact of membrane lipid composition on the structure and stability of the transmembrane domain of amyloid precursor protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E5281-7.	7.1	74
103	Multiple Probes are Required to Explore and Control the Rugged Energy Landscape of RNA Hairpins. <i>Journal of the American Chemical Society</i> , 2008, 130, 1538-1539.	13.7	73
104	Dissecting the Kinematics of the Kinesin Step. <i>Structure</i> , 2012, 20, 628-640.	3.3	73
105	Structures and Free-Energy Landscapes of the Wild Type and Mutants of the A β 21-30 Peptide Are Determined by an Interplay between Intrapeptide Electrostatic and Hydrophobic Interactions. <i>Journal of Molecular Biology</i> , 2008, 379, 815-829.	4.2	71
106	Denaturant-dependent folding of GFP. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 17832-17838.	7.1	71
107	Chain organization of human interphase chromosome determines the spatiotemporal dynamics of chromatin loci. <i>PLoS Computational Biology</i> , 2018, 14, e1006617.	3.2	71
108	Mean-field Potts glass model: Initial-condition effects on dynamics and properties of metastable states. <i>Physical Review B</i> , 1988, 38, 4881-4892.	3.2	70

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109	Semiflexible chains under tension. <i>Journal of Chemical Physics</i> , 1997, 106, 4243-4247.	3.0	70
110	Allosteric Communication in Dihydrofolate Reductase: Signaling Network and Pathways for Closed to Occluded Transition and Back. <i>Journal of Molecular Biology</i> , 2007, 374, 250-266.	4.2	69
111	Charge states rather than propensity for β^2 -structure determine enhanced fibrillogenesis in wild-type Alzheimer's β^2 -amyloid peptide compared to E22Q Dutch mutant. <i>Protein Science</i> , 2009, 11, 1639-1647.	7.6	69
112	Confinement-Induced Glassy Dynamics in a Model for Chromosome Organization. <i>Physical Review Letters</i> , 2015, 115, 198102.	7.8	69
113	RNA Tertiary Interactions Mediate Native Collapse of a Bacterial Group I Ribozyme. <i>Journal of Molecular Biology</i> , 2005, 353, 1199-1209.	4.2	66
114	A mean-field model for semiflexible chains. <i>Journal of Chemical Physics</i> , 1995, 103, 9408-9412.	3.0	63
115	Time Scales for the Formation of the Most Probable Tertiary Contacts in Proteins with Applications to Cytochrome c. <i>Journal of Physical Chemistry B</i> , 1999, 103, 608-610.	2.6	61
116	Kinetics of interior loop formation in semiflexible chains. <i>Journal of Chemical Physics</i> , 2006, 124, 104905.	3.0	61
117	Promoter melting triggered by bacterial RNA polymerase occurs in three steps. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 12523-12528.	7.1	61
118	Extracting Stacking Interaction Parameters for RNA from the Data Set of Native Structures. <i>Journal of Molecular Biology</i> , 2005, 347, 53-69.	4.2	60
119	Rigor to Post-Rigor Transition in Myosin V: Link between the Dynamics and the Supporting Architecture. <i>Structure</i> , 2010, 18, 471-481.	3.3	60
120	Theoretical perspectives on biological machines. <i>Reviews of Modern Physics</i> , 2020, 92, .	45.6	60
121	Counterion Charge Density Determines the Position and Plasticity of RNA Folding Transition States. <i>Journal of Molecular Biology</i> , 2006, 359, 446-454.	4.2	59
122	Force-dependent switch in protein unfolding pathways and transition-state movements. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E715-24.	7.1	59
123	Free polymer in a colloidal solution. <i>Physical Review A</i> , 1991, 44, R4797-R4800.	2.5	57
124	Virtual atom representation of hydrogen bonds in minimal off-lattice models of β^2 helices: effect on stability, cooperativity and kinetics. <i>Folding & Design</i> , 1998, 3, 481-496.	4.5	57
125	Molecular Origin of Constant $\langle i \rangle_m \langle i \rangle$ -Values, Denatured State Collapse, and Residue-Dependent Transition Midpoints in Globular Proteins. <i>Biochemistry</i> , 2009, 48, 3743-3754.	2.5	56
126	Conformations of a polyelectrolyte chain. <i>Physical Review A</i> , 1992, 46, R3012-R3015.	2.5	55

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127	Propensity to Form Amyloid Fibrils Is Encoded as Excitations in the Free Energy Landscape of Monomeric Proteins. <i>Journal of Molecular Biology</i> , 2014, 426, 2653-2666.	4.2	55
128	Theory and simulations for RNA folding in mixtures of monovalent and divalent cations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 21022-21030.	7.1	55
129	Order-disorder transition in colloidal suspensions. <i>Physical Review A</i> , 1987, 36, 5690-5700.	2.5	54
130	Are disordered spin glass models relevant for the structural glass problem?. <i>Transport Theory and Statistical Physics</i> , 1995, 24, 927-945.	0.4	54
131	Charge fluctuation effects on the shape of flexible polyampholytes with applications to intrinsically disordered proteins. <i>Journal of Chemical Physics</i> , 2018, 149, 163323.	3.0	54
132	Finite Size Effects on Thermal Denaturation of Globular Proteins. <i>Physical Review Letters</i> , 2004, 93, 268107.	7.8	53
133	Native secondary structure formation in RNA may be a slave to tertiary folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1998, 95, 11506-11508.	7.1	52
134	Protein folding: from theory to practice. <i>Current Opinion in Structural Biology</i> , 2013, 23, 22-29.	5.7	52
135	Molecular-dynamics study of glassy and supercooled states of a binary mixture of soft spheres. <i>Physical Review A</i> , 1987, 36, 3300-3311.	2.5	50
136	Persistence length of flexible polyelectrolyte chains. <i>Journal of Chemical Physics</i> , 1999, 110, 7533-7541.	3.0	50
137	Symmetric Connectivity of Secondary Structure Elements Enhances the Diversity of Folding Pathways. <i>Journal of Molecular Biology</i> , 2005, 353, 1171-1186.	4.2	50
138	Phenomenological and microscopic theories for catch bonds. <i>Journal of Structural Biology</i> , 2017, 197, 50-56.	2.8	50
139	Differences in the free energies between the excited states of A $\langle i \rangle^{\hat{1}^2} \langle j \rangle^{\hat{1}^2}$ 40 and A $\langle i \rangle^{\hat{1}^2} \langle j \rangle^{\hat{1}^2}$ 42 monomers encode their aggregation propensities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 19926-19937.	7.1	49
140	Interactions between amino acid side chains in cylindrical hydrophobic nanopores with applications to peptide stability. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 17636-17641.	7.1	47
141	Coupling between Normal Modes Drives Protein Conformational Dynamics: Illustrations Using Allosteric Transitions in Myosin II. <i>Biophysical Journal</i> , 2009, 96, 2128-2137.	0.5	47
142	Folding of Human Telomerase RNA Pseudoknot Using Ion-Jump and Temperature-Quench Simulations. <i>Journal of the American Chemical Society</i> , 2011, 133, 20634-20643.	13.7	47
143	Chain Length Determines the Folding Rates of RNA. <i>Biophysical Journal</i> , 2012, 102, L11-L13.	0.5	47
144	Maximizing RNA folding rates: A balancing act. <i>Rna</i> , 2000, 6, 790-794.	3.5	46

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145	Theory of the Molecular Transfer Model for Proteins with Applications to the Folding of the src-SH3 Domain. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6707-6716.	2.6	46
146	Design principles governing the motility of myosin V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, E4059-E4068.	7.1	46
147	Plasticity of hydrogen bond networks regulates mechanochemistry of cell adhesion complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 9048-9053.	7.1	46
148	Sequence-Dependent Three Interaction Site Model for Single- and Double-Stranded DNA. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3763-3779.	5.3	46
149	Dissecting Ubiquitin Folding Using the Self-Organized Polymer Model. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11358-11370.	2.6	45
150	Internal Constraints Induce Localization in an Isolated Polymer Molecule. <i>Physical Review Letters</i> , 1996, 76, 542-545.	7.8	43
151	Allosteric Transitions in Biological Nanomachines are Described by Robust Normal Modes of Elastic Networks. <i>Current Protein and Peptide Science</i> , 2009, 10, 128-132.	1.4	43
152	Ultrasensitivity of Water Exchange Kinetics to the Size of Metal Ion. <i>Journal of the American Chemical Society</i> , 2017, 139, 12334-12337.	13.7	43
153	Structural Heterogeneity in Transmembrane Amyloid Precursor Protein Homodimer Is a Consequence of Environmental Selection. <i>Journal of the American Chemical Society</i> , 2014, 136, 9619-9626.	13.7	40
154	Stretching Homopolymers. <i>Macromolecules</i> , 2007, 40, 7343-7353.	4.8	39
155	Factors Governing Helix Formation in Peptides Confined to Carbon Nanotubes. <i>Nano Letters</i> , 2008, 8, 3702-3708.	9.1	38
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