Xuhui Huang

List of Publications by Year in Descending Order

142 papers	7,857 citations	48 h-index	87 g-index
152 ext. papers	9,105 ext. citations	9.4 avg, IF	6.09 L-index

#	Paper	IF	Citations
142	Elucidation of the key role of Pt⋯Pt interactions in the directional self-assembly of platinum(II) complexes.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2116543119	11.5	2
141	Critical role of backbone coordination in the mRNA recognition by RNA induced silencing complex. *Communications Biology*, **2021**, 4, 1345	6.7	2
140	Role of bacterial RNA polymerase gate opening dynamics in DNA loading and antibiotics inhibition elucidated by quasi-Markov State Model. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	7
139	Transcriptional processing of an unnatural base pair by eukaryotic RNA polymerase II. *Nature Chemical Biology*, **2021**, 17, 906-914	11.7	5
138	Are endoplasmic reticulum subdomains shaped by asymmetric distribution of phospholipids? Evidence from a C. elegans model system. *BioEssays*, **2021**, 43, e2000199	4.1	2
137	Elucidating molecular mechanisms of functional conformational changes of proteins via Markov state models. *Current Opinion in Structural Biology*, **2021**, 67, 69-77	8.1	7
136	Entropy of stapled peptide inhibitors in free state is the major contributor to the improvement of binding affinity with the GK domain. *RSC Chemical Biology*, **2021**, 2, 1274-1284	3	2
135	Incorporation efficiency and inhibition mechanism of 2'-substituted nucleotide analogs against SARS-CoV-2 RNA-dependent RNA polymerase. *Physical Chemistry Chemical Physics*, **2021**, 23, 20117-20128	3.6	3
134	Construction of diverse peptide structural architectures chemoselective peptide ligation. *Chemical Science*, **2021**, 12, 7091-7097	9.4	3
133	Microsecond timescale MD simulations at the transition state of HMGR predict remote allosteric residues. *Chemical Science*, **2021**, 12, 6413-6418	9.4	3
132	A comprehensive mechanism for 5-carboxylcytosine-induced transcriptional pausing revealed by Markov state models. *Journal of Biological Chemistry*, **2021**, 296, 100735	5.4	
131	Role of Surface Templating on Ice Nucleation Efficiency on a Silver Iodide Surface. *Journal of Physical Chemistry C*, **2021**, 125, 18857-18865	3.8	1
130	A novel mechanism of enhanced transcription activity and fidelity for influenza A viral RNA-dependent RNA polymerase. *Nucleic Acids Research*, **2021**, 49, 8796-8810	20.1	2
129	Temperature-dependent kinetic pathways of heterogeneous ice nucleation competing between classical and non-classical nucleation. *Nature Communications*, **2021**, 12, 4954	17.4	2
128	Markov State Models to Study the Functional Dynamics of Proteins in the Wake of Machine Learning. *Jacs Au*, **2021**, 1, 1330-1341		4
127	The mechanism of action of T-705 as a unique delayed chain terminator on influenza viral polymerase transcription. *Biophysical Chemistry*, **2021**, 277, 106652	3.5	1
126	1'-Ribose cyano substitution allows Remdesivir to effectively inhibit nucleotide addition and proofreading during SARS-CoV-2 viral RNA replication. *Physical Chemistry Chemical Physics*, **2021**, 23, 5852-5863	3.6	13

125	Molecular basis defining the selectivity of substituted isoquinolinones for the melatonin MT receptor. *Biochemical Pharmacology*, **2020**, 177, 114020	6	3
124	On the advantages of exploiting memory in Markov state models for biomolecular dynamics. *Journal of Chemical Physics*, **2020**, 153, 014105	3.9	7
123	The hydrolytic water molecule of Class A ß-lactamase relies on the acyl-enzyme intermediate ES* for proper coordination and catalysis. *Scientific Reports*, **2020**, 10, 10205	4.9	6
122	Three-site and five-site fixed-charge water models compatible with AMOEBA force field. *Journal of Computational Chemistry*, **2020**, 41, 1034-1044	3.5	2
121	Remdesivir, lopinavir, emetine, and homoharringtonine inhibit SARS-CoV-2 replication in vitro. *Antiviral Research*, **2020**, 178, 104786	10.8	528
120	Identifying Transcription Error-Enriched Genomic Loci Using Nuclear Run-on Circular-Sequencing Coupled with Background Error Modeling. *Journal of Molecular Biology*, **2020**, 432, 3933-3949	6.5	2
119	Target search and recognition mechanisms of glycosylase AlkD revealed by scanning FRET-FCS and Markov state models. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 21889-21895	11.5	9
118	A theoretical study on the dynamics of light harvesting in the dimeric photosystem II core complex: regulation and robustness of energy transfer pathways. *Faraday Discussions*, **2019**, 216, 94-115	3.6	8
117	Recent Developments in Integral Equation Theory for Solvation to Treat Density Inhomogeneity at Solute–Solvent Interface. *Advanced Theory and Simulations*, **2019**, 2, 1900049	3.5	4
116	Mechanistic Insights and Rational Design of a Versatile Surface with Cells/Bacteria Recognition Capability via Orientated Fusion Peptides. *Advanced Science*, **2019**, 6, 1801827	13.6	9
115	TAPS: A traveling-salesman based automated path searching method for functional conformational changes of biological macromolecules. *Journal of Chemical Physics*, **2019**, 150, 124105	3.9	8
114	8-Oxo-guanine DNA damage induces transcription errors by escaping two distinct fidelity control checkpoints of RNA polymerase II. *Journal of Biological Chemistry*, **2019**, 294, 4924-4933	5.4	2
113	Intrinsic Cleavage of RNA Polymerase II Adopts a Nucleobase-independent Mechanism Assisted by Transcript Phosphate. *Nature Catalysis*, **2019**, 2, 228-235	36.5	8
112	Specific and Quantitative Detection of Albumin in Biological Fluids by Tetrazolate-Functionalized Water-Soluble AIEgens. *ACS Applied Materials & Interfaces*, **2019**, 11, 29619-29629	9.5	26
111	Non-aromatic annulene-based aggregation-induced emission system via aromaticity reversal process. *Nature Communications*, **2019**, 10, 2952	17.4	79
110	A deep learning framework to predict binding preference of RNA constituents on protein surface. *Nature Communications*, **2019**, 10, 4941	17.4	25
109	Two symmetric arginine residues play distinct roles in Argonaute DNA guide strand-mediated DNA target cleavage. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 845-853	11.5	10
108	Allosteric Effector ppGpp Potentiates the Inhibition of Transcript Initiation by DksA. *Molecular Cell*, **2018**, 69, 828-839.e5	17.6	66

107	Molecular mechanisms of RNA polymerase II transcription elongation elucidated by kinetic network models. *Current Opinion in Structural Biology*, **2018**, 49, 54-62	8.1	11
106	Harnessing complexity in molecular self-assembly using computer simulations. *Physical Chemistry Chemical Physics*, **2018**, 20, 6767-6776	3.6	6
105	3DRISM-HI-D2MSA: an improved analytic theory to compute solvent structure around hydrophobic solutes with proper treatment of solute□solvent electrostatic interactions. *Molecular Physics*, **2018**, 116, 1003-1013	1.7	2
104	Mechanochromism: Multifunctional AIEgens: Ready Synthesis, Tunable Emission, Mechanochromism, Mitochondrial, and Bacterial Imaging (Adv. Funct. Mater. 1/2018). *Advanced Functional Materials*, **2018**, 28, 1870006	15.6	
103	Improving the productivity of monodisperse polyhedral cages by the rational design of kinetic self-assembly pathways. *Physical Chemistry Chemical Physics*, **2018**, 20, 10030-10037	3.6	1
102	Constructing Markov State Models to elucidate the functional conformational changes of complex biomolecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1343	7.9	49
101	Identification of new EphA4 inhibitors by virtual screening of FDA-approved drugs. *Scientific Reports*, **2018**, 8, 7377	4.9	12
100	White-Light Emission of a Binary Light-Harvesting Platform Based on an Amphiphilic Organic Cage. *Chemistry of Materials*, **2018**, 30, 1285-1290	9.6	77
99	Structural dissection of an interaction between transcription initiation and termination factors implicated in promoter-terminator cross-talk. *Journal of Biological Chemistry*, **2018**, 293, 1651-1665	5.4	9
98	Multifunctional AIEgens: Ready Synthesis, Tunable Emission, Mechanochromism, Mitochondrial, and Bacterial Imaging. *Advanced Functional Materials*, **2018**, 28, 1704589	15.6	84
97	Clustering algorithms to analyze molecular dynamics simulation trajectories for complex chemical and biological systems□*Chinese Journal of Chemical Physics*, **2018**, 31, 404-420	0.9	14
96	DATA-DRIVEN TIGHT FRAME FOR CRYO-EM IMAGE DENOISING AND CONFORMATIONAL CLASSIFICATION **2018**,		4
95	DNA-Encoded Dynamic Chemical Library and Its Applications in Ligand Discovery. *Journal of the American Chemical Society*, **2018**, 140, 15859-15867	16.4	59
94	An efficient Bayesian kinetic lumping algorithm to identify metastable conformational states via Gibbs sampling. *Journal of Chemical Physics*, **2018**, 149, 072337	3.9	8
93	Crystallographic Snapshots of Class A β-Lactamase Catalysis Reveal Structural Changes That Facilitate β-Lactam Hydrolysis. *Journal of Biological Chemistry*, **2017**, 292, 4022-4033	5.4	16
92	Maltose-binding protein effectively stabilizes the partially closed conformation of the ATP-binding cassette transporter MalFGK. *Physical Chemistry Chemical Physics*, **2017**, 19, 9366-9373	3.6	7
91	Single-Molecule Investigations of Conformation Adaptation of Porphyrins on Surfaces. *Journal of Physical Chemistry Letters*, **2017**, 8, 1241-1247	6.4	17
90	Ca-Induced Rigidity Change of the Myosin VIIa IQ Motif-Single α-Helix Lever Arm Extension. *Structure*, **2017**, 25, 579-591.e4	5.2	15

89	AIEgen-based theranostic system: targeted imaging of cancer cells and adjuvant amplification of antitumor efficacy of paclitaxel. *Chemical Science*, **2017**, 8, 2191-2198	9.4	91
88	Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. *Nature Communications*, **2017**, 8, 15639	17.4	47
87	Kinetics-Controlled Amphiphile Self-Assembly Processes. *Journal of Physical Chemistry Letters*, **2017**, 8, 1798-1803	6.4	14
86	Elucidating Mechanisms of Molecular Recognition Between Human Argonaute and miRNA Using Computational Approaches. *Methods in Molecular Biology*, **2017**, 1517, 251-275	1.4	
85	Massively parallel de novo protein design for targeted therapeutics. *Nature*, **2017**, 550, 74-79	50.4	235
84	Why Do Simple Molecules with "Isolated" Phenyl Rings Emit Visible Light?. *Journal of the American Chemical Society*, **2017**, 139, 16264-16272	16.4	130
83	Achieving enhanced cell penetration of short conformationally constrained peptides through amphiphilicity tuning. *Chemical Science*, **2017**, 8, 7576-7581	9.4	29
82	Path lumping: An efficient algorithm to identify metastable path channels for conformational dynamics of multi-body systems. *Journal of Chemical Physics*, **2017**, 147, 044112	3.9	5
81	Unique Roles of the Non-identical MCM Subunits in DNA Replication Licensing. *Molecular Cell*, **2017**, 67, 168-179	17.6	31
80	Dramatic Differences in Aggregation-Induced Emission and Supramolecular Polymerizability of Tetraphenylethene-Based Stereoisomers. *Journal of the American Chemical Society*, **2017**, 139, 10150-10158	16.4	121
79	Understanding the core of RNA interference: The dynamic aspects of Argonaute-mediated processes. *Progress in Biophysics and Molecular Biology*, **2017**, 128, 39-46	4.7	7
78	Adaptive partitioning by local density-peaks: An efficient density-based clustering algorithm for analyzing molecular dynamics trajectories. *Journal of Computational Chemistry*, **2017**, 38, 152-160	3.5	21
77	Synaptic Targeting and Function of SAPAPs Mediated by Phosphorylation-Dependent Binding to PSD-95 MAGUKs. *Cell Reports*, **2017**, 21, 3781-3793	10.6	29
76	Synthesis, optical properties, and helical self-assembly of a bivaline-containing tetraphenylethene. *Scientific Reports*, **2016**, 6, 19277	4.9	53
75	Functional interplay between NTP leaving group and base pair recognition during RNA polymerase II nucleotide incorporation revealed by methylene substitution. *Nucleic Acids Research*, **2016**, 44, 3820-8	20.1	4
74	Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. *Nanoscale*, **2016**, 8, 15173-80	7.7	77
73	Elucidation of the conformational dynamics of multi-body systems by construction of Markov state models. *Physical Chemistry Chemical Physics*, **2016**, 18, 30228-30235	3.6	14
72	Elucidation of the Dynamics of Transcription Elongation by RNA Polymerase II using Kinetic Network Models. *Accounts of Chemical Research*, **2016**, 49, 687-94	24.3	30

71	A Flexible Domain-Domain Hinge Promotes an Induced-fit Dominant Mechanism for the Loading of Guide-DNA into Argonaute Protein in Thermus thermophilus. *Journal of Physical Chemistry B*, **2016**, 120, 2709-20	3.4	17
70	Stapling of unprotected helical peptides photo-induced intramolecular thiol-yne hydrothiolation. *Chemical Science*, **2016**, 7, 3325-3330	9.4	61
69	Controlling the Integration of Polyvinylpyrrolidone onto Substrate by Quartz Crystal Microbalance with Dissipation To Achieve Excellent Protein Resistance and Detoxification. *ACS Applied Materials & Interfaces*, **2016**, 8, 18684-92	9.5	11
68	Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. *Angewandte Chemie*, **2016**, 128, 14196-14200	3.6	3
67	Enhancing pairwise state-transition weights: A new weighting scheme in simulated tempering that can minimize transition time between a pair of conformational states. *Journal of Chemical Physics*, **2016**, 144, 154107	3.9	1
66	Bridge helix bending promotes RNA polymerase II backtracking through a critical and conserved threonine residue. *Nature Communications*, **2016**, 7, 11244	17.4	54
65	Elucidating dominant pathways of the nano-particle self-assembly process. *Physical Chemistry Chemical Physics*, **2016**, 18, 23494-9	3.6	11
64	Constructing Kinetic Network Models to Elucidate Mechanisms of Functional Conformational Changes of Enzymes and Their Recognition with Ligands. *Methods in Enzymology*, **2016**, 578, 343-71	1.7	3
63	Dynamics of the conformational transitions during the dimerization of an intrinsically disordered peptide: a case study on the human islet amyloid polypeptide fragment. *Physical Chemistry Chemical Physics*, **2016**, 18, 29892-29904	3.6	12
62	Conformational Dynamics of apo-GlnBP Revealed by Experimental and Computational Analysis. *Angewandte Chemie - International Edition*, **2016**, 55, 13990-13994	16.4	26
61	Reduced Intramolecular Twisting Improves the Performance of 3D Molecular Acceptors in Non-Fullerene Organic Solar Cells. *Advanced Materials*, **2016**, 28, 8546-8551	24	143
60	Impact of template backbone heterogeneity on RNA polymerase II transcription. *Nucleic Acids Research*, **2015**, 43, 2232-41	20.1	12
59	Reference interaction site model with hydrophobicity induced density inhomogeneity: An analytical theory to compute solvation properties of large hydrophobic solutes in the mixture of polyatomic solvent molecules. *Journal of Chemical Physics*, **2015**, 143, 054110	3.9	6
58	The influence of spacer units on molecular properties and solar cell performance of non-fullerene acceptors. *Journal of Materials Chemistry A*, **2015**, 3, 20108-20112	13	36
57	Automatic state partitioning for multibody systems (APM): an efficient algorithm for constructing Markov state models to elucidate conformational dynamics of multibody systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 17-27	6.4	29
56	A tetraphenylethylene core-based 3D structure small molecular acceptor enabling efficient non-fullerene organic solar cells. *Advanced Materials*, **2015**, 27, 1015-20	24	334
55	Aggregation-Induced-Emission-Active Macrocycle Exhibiting Analogous Triply and Singly Twisted MÖbius Topologies. *Chemistry - A European Journal*, **2015**, 21, 11707-11	4.8	13
54	Structural Model of RNA Polymerase II Elongation Complex with Complete Transcription Bubble Reveals NTP Entry Routes. *PLoS Computational Biology*, **2015**, 11, e1004354	5	9

53	Mechanism of action of thalassospiramides, a new class of calpain inhibitors. *Scientific Reports*, **2015**, 5, 8783	4.9	13
52	Poly[(maleic anhydride)-alt-(vinyl acetate)]: A Pure Oxygenic Nonconjugated Macromolecule with Strong Light Emission and Solvatochromic Effect. *Macromolecules*, **2015**, 48, 64-71	5.5	183
51	Organic Solar Cells: A Tetraphenylethylene Core-Based 3D Structure Small Molecular Acceptor Enabling Efficient Non-Fullerene Organic Solar Cells (Adv. Mater. 6/2015). *Advanced Materials*, **2015**, 27, 1014-1014	24	8
50	Markov State Models Reveal a Two-Step Mechanism of miRNA Loading into the Human Argonaute Protein: Selective Binding followed by Structural Re-arrangement. *PLoS Computational Biology*, **2015**, 11, e1004404	5	39
49	Dynamic protein conformations preferentially drive energy transfer along the active chain of the photosystem II reaction centre. *Nature Communications*, **2014**, 5, 4170	17.4	33
48	Constructing kinetic models to elucidate structural dynamics of a complete RNA polymerase II elongation cycle. *Physical Biology*, **2014**, 12, 016004	3	10
47	Strand-specific (asymmetric) contribution of phosphodiester linkages on RNA polymerase II transcriptional efficiency and fidelity. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, E3269-76	11.5	8
46	Blockade of EphA4 signaling ameliorates hippocampal synaptic dysfunctions in mouse models of Alzheimer's disease. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 9959-64	11.5	127
45	Quantitatively characterizing the ligand binding mechanisms of choline binding protein using Markov state model analysis. *PLoS Computational Biology*, **2014**, 10, e1003767	5	55
44	Millisecond dynamics of RNA polymerase II translocation at atomic resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 7665-70	11.5	90
43	Application of Markov State Models to simulate long timescale dynamics of biological macromolecules. *Advances in Experimental Medicine and Biology*, **2014**, 805, 29-66	3.6	22
42	Understanding molecular recognition by kinetic network models constructed from molecular dynamics simulations. *Advances in Experimental Medicine and Biology*, **2014**, 797, 107-14	3.6	3
41	Quantitative comparison of alternative methods for coarse-graining biological networks. *Journal of Chemical Physics*, **2013**, 139, 121905	3.9	42
40	Dynamics of an intrinsically disordered protein reveal metastable conformations that potentially seed aggregation. *Journal of the American Chemical Society*, **2013**, 135, 16092-101	16.4	125
39	A fast parallel clustering algorithm for molecular simulation trajectories. *Journal of Computational Chemistry*, **2013**, 34, 95-104	3.5	25
38	A two-state model for the dynamics of the pyrophosphate ion release in bacterial RNA polymerase. *PLoS Computational Biology*, **2013**, 9, e1003020	5	40
37	Hierarchical Nyström methods for constructing Markov state models for conformational dynamics. *Journal of Chemical Physics*, **2013**, 138, 174106	3.9	37
36	THEORETICAL INVESTIGATIONS ON ELUCIDATING FUNDAMENTAL MECHANISMS OF CATALYSIS AND DYNAMICS INVOLVED IN TRANSCRIPTION BY RNA POLYMERASE. *Journal of Theoretical and Computational Chemistry*, **2013**, 12, 1341005	1.8	4

35	Monitoring and inhibition of insulin fibrillation by a small organic fluorogen with aggregation-induced emission characteristics. *Journal of the American Chemical Society*, **2012**, 134, 1680-9	16.4	293
34	Dynamics of pyrophosphate ion release and its coupled trigger loop motion from closed to open state in RNA polymerase II. *Journal of the American Chemical Society*, **2012**, 134, 2399-406	16.4	94
33	Investigating the structural origin of trpzip2 temperature dependent unfolding fluorescence line shape based on a Markov state model simulation. *Journal of Physical Chemistry B*, **2012**, 116, 12669-76	3.4	10
32	Bridging the Gap Between Optical Spectroscopic Experiments and Computer Simulations for Fast Protein Folding Dynamics. *Current Physical Chemistry*, **2012**, 2, 45-58	0.5	4
31	Multiscale modeling of macromolecular biosystems. *Briefings in Bioinformatics*, **2012**, 13, 395-405	13.4	23
30	Force field development for cofactors in the photosystem II. *Journal of Computational Chemistry*, **2012**, 33, 1969-80	3.5	40
29	What makes efficient circularly polarised luminescence in the condensed phase: aggregation-induced circular dichroism and light emission. *Chemical Science*, **2012**, 3, 2737	9.4	297
28	Initiation complex structure and promoter proofreading. *Science*, **2011**, 333, 633-7	33.3	48
27	Simulating the T-jump-triggered unfolding dynamics of trpzip2 peptide and its time-resolved IR and two-dimensional IR signals using the Markov state model approach. *Journal of Physical Chemistry B*, **2011**, 115, 5415-24	3.4	59
26	Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation. *Rna*, **2011**, 17, 1066-75	5.8	67
25	A role for both conformational selection and induced fit in ligand binding by the LAO protein. *PLoS Computational Biology*, **2011**, 7, e1002054	5	172
24	RNA polymerase II trigger loop residues stabilize and position the incoming nucleotide triphosphate in transcription. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 15745-50	11.5	53
23	X-ray structure and mechanism of RNA polymerase II stalled at an antineoplastic monofunctional platinum-DNA adduct. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 9584-9	11.5	105
22	Network models for molecular kinetics and their initial applications to human health. *Cell Research*, **2010**, 20, 622-30	24.7	41
21	Constructing multi-resolution Markov State Models (MSMs) to elucidate RNA hairpin folding mechanisms. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2010**, 228-39	1.3	33
20	Dewetting transitions in protein cavities. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 1856-69	4.2	60
19	Topological methods for exploring low-density states in biomolecular folding pathways. *Journal of Chemical Physics*, **2009**, 130, 144115	3.9	82
18	Using generalized ensemble simulations and Markov state models to identify conformational states. *Methods*, **2009**, 49, 197-201	4.6	227

17	The predicted structure of the headpiece of the Huntingtin protein and its implications on Huntingtin aggregation. *Journal of Molecular Biology*, **2009**, 388, 919-27	6.5	62
16	Rapid equilibrium sampling initiated from nonequilibrium data. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 19765-9	11.5	115
15	Adaptive Seeding: A New Method for Simulating Biologically Relevant Timescales. *Biophysical Journal*, **2009**, 96, 575a	2.9	2
14	Structural basis of transcription: backtracked RNA polymerase II at 3.4 angstrom resolution. *Science* , **2009**, 324, 1203-6	33.3	195
13	Structural insight into RNA hairpin folding intermediates. *Journal of the American Chemical Society*, **2008**, 130, 9676-8	16.4	83
12	Molecular dynamics study of the temperature-dependent Optical Kerr effect spectra and intermolecular dynamics of room temperature ionic liquid 1-methoxyethylpyridinium dicyanoamide. *Journal of Physical Chemistry B*, **2008**, 112, 7837-49	3.4	77
11	Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. *Journal of Chemical Physics*, **2008**, 128, 205106	3.9	56
10	Nanoscale dewetting transition in protein complex folding. *Journal of Physical Chemistry B*, **2007**, 111, 9069-77	3.4	72
9	Replica exchange with solute tempering: efficiency in large scale systems. *Journal of Physical Chemistry B*, **2007**, 111, 5405-10	3.4	95
8	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. *Journal of Physical Chemistry B*, **2006**, 110, 19018-22	3.4	71
7	Dynamics of water confined in the interdomain region of a multidomain protein. *Journal of Physical Chemistry B*, **2006**, 110, 3704-11	3.4	88
6	Drying and hydrophobic collapse of paraffin plates. *Journal of Physical Chemistry B*, **2005**, 109, 3546-52	3.4	65
5	Why is the partial molar volume of CO2 so small when dissolved in a room temperature ionic liquid? Structure and dynamics of CO2 dissolved in [Bmim+] [PF6(-)]. *Journal of the American Chemical Society*, **2005**, 127, 17842-51	16.4	307
4	Observation of a dewetting transition in the collapse of the melittin tetramer. *Nature*, **2005**, 437, 159-62	50.4	333
3	Hydrophobic collapse in multidomain protein folding. *Science*, **2004**, 305, 1605-9	33.3	441
2	Dewetting-induced collapse of hydrophobic particles. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 11953-8	11.5	245
1	Role of 1′-Ribose Cyano Substitution for Remdesivir to Effectively Inhibit Nucleotide Addition and Proofreading in SARS-CoV-2 Viral RNA Replication		6