Lijiang Yang

List of Publications by Year
in descending order

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51 papers	1,948 citations	255252 23 h-index	247751 42 g-index
53 all docs	53 docs citations	53 times ranked	2804 citing authors

#	Article	IF	Citations
1	<scp>SPONGE</scp>: A <scp>GPUâ€Accelerated</scp> Molecular Dynamics Package with Enhanced Sampling and <scp>Alâ€Driven</scp> Algorithms. Chinese Journal of Chemistry, 2022, 40, 160-168.	6.5	15
2	Two-step fitness selection for intra-host variations in SARS-CoV-2. Cell Reports, 2022, 38, 110205.	6.3	42
3	Enhanced Sampling Simulation Reveals How Solvent Influences Chirogenesis of the Intra-Molecular Dielsâ€“Alder Reaction. Journal of Chemical Theory and Computation, 2022, 18, 4318-4326.	5.5	6
4	Deep reinforcement learning of transition states. Physical Chemistry Chemical Physics, 2021, 23, 6888-6895.	2.9	22
5	A perspective on the molecular simulation of DNA from structural and functional aspects. Chemical Science, 2021, 12, 5390-5409.	7.7	14
6	Comparison of the Microsolvation of CaX₂ (X = F, Cl, Br, I) in Water: Size-Selected Anion Photoelectron Spectroscopy and Theoretical Calculations. Journal of Physical Chemistry A, 2021, 125, 3288-3306.	2.6	6
7	A Perspective on Deep Learning for Molecular Modeling and Simulations. Journal of Physical Chemistry A, 2020, 124, 6745-6763.	2.6	39
8	Hydration processes of barium chloride: Size-selected anion photoelectron spectroscopy and theoretical calculations of BaCl2-water clusters. Journal of Chemical Physics, 2020, 153, 134301.	3.0	5
9	Role of Engineered Iron-haem Enzyme in Reactivity and Stereoselectivity of Intermolecular Benzylic Câ€“H Bond Amination. ACS Catalysis, 2020, 10, 5318-5327.	11.5	26
10	Enhanced sampling in molecular dynamics. Journal of Chemical Physics, 2019, 151, 070902.	3.0	273
11	The Exploration of a New Stable G-Triplex DNA and Its Novel Function in Electrochemical Biosensing. Analytical Chemistry, 2019, 91, 10731-10737.	6.7	24
12	Structure of water confined between two parallel graphene plates. Journal of Chemical Physics, 2019, 150, 124703.	3.0	34
13	CDNsâ€“STING Interaction Mechanism Investigations and Instructions on Design of CDN-Derivatives. Journal of Physical Chemistry B, 2018, 122, 1862-1868.	2.7	12
14	Role of Conformational Fluctuations of Protein toward Methylation in DNA by Cytosine-5-methyltransferase. Journal of Chemical Theory and Computation, 2018, 14, 6679-6689.	5.5	3
15	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. Journal of Chemical Theory and Computation, 2018, 14, 5787-5796.	5.5	24
16	Microscopic Insight into the Protein Denaturation Action of Urea and Its Methyl Derivatives. Journal of Physical Chemistry Letters, 2018, 9, 2933-2940.	4.8	12
17	From 1D sequence to 3D chromatin dynamics and cellular functions: a phase separation perspective. Nucleic Acids Research, 2018, 46, 9367-9383.	13.9	56
18	Molecular dynamics simulation, ab initio calculation, and size-selected anion photoelectron spectroscopy study of initial hydration processes of calcium chloride. Journal of Chemical Physics, 2018, 148, 222839.	3.0	14

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19	Single Mutations Reshape the Structural Correlation Network of the DMXAAâ€“Human STING Complex. Journal of Physical Chemistry B, 2017, 121, 2073-2082.	2.7	15
20	Polarization Effects on the Cellulose Dissolution in Ionic Liquids: Molecular Dynamics Simulations with Polarization Model and Integrated Tempering Enhanced Sampling Method. Journal of Physical Chemistry B, 2017, 121, 4319-4332.	2.7	10
21	Rich Dynamics Underlying Solution Reactions Revealed by Sampling and Data Mining of Reactive Trajectories. ACS Central Science, 2017, 3, 407-414.	12.1	14
22	Efficient sampling over rough energy landscapes with high barriers: A combination of metadynamics with integrated tempering sampling. Journal of Chemical Physics, 2016, 144, 094105.	3.0	26
23	Conformation switching of AIM2 PYD domain revealed by NMR relaxation and MD simulation. Biochemical and Biophysical Research Communications, 2016, 473, 636-641.	2.2	9
24	Structural Flexibility and Conformation Features of Cyclic Dinucleotides in Aqueous Solutions. Journal of Physical Chemistry B, 2016, 120, 2670-2680.	2.7	11
25	Accurate placement of substrate RNA by Gar1 in H/ACA RNA-guided pseudouridylation. Nucleic Acids Research, 2015, 43, 7207-7216.	13.9	16
26	Conformational Preadjustment in Aqueous Claisen Rearrangement Revealed by SITS-QM/MM MD Simulations. Journal of Physical Chemistry B, 2015, 119, 5518-5530.	2.7	18
27	From Thermodynamics to Kinetics: Enhanced Sampling of Rare Events. Accounts of Chemical Research, 2015, 48, 947-955.	16.2	67
28	Dynamics and Kinetics Study of â€œIn-Waterâ€•Chemical Reactions by Enhanced Sampling of Reactive Trajectories. Journal of Physical Chemistry B, 2015, 119, 14505-14514.	2.7	22
29	DNA Structural Correlation in Short and Long Ranges. Journal of Physical Chemistry B, 2015, 119, 13980-13990.	2.7	22
30	Combine umbrella sampling with integrated tempering method for efficient and accurate calculation of free energy changes of complex energy surface. Journal of Chemical Physics, 2014, 141, 044108.	3.0	27
31	Discriminating trpzip2 and trpzip4 peptidesâ€™ folding landscape using the two-dimensional infrared spectroscopy: A simulation study. Journal of Chemical Physics, 2014, 140, 055101.	3.0	10
32	On the molecular mechanism of ion specific Hofmeister series. Science China Chemistry, 2014, 57, 36-47.	8.7	19
33	How Quickly Can a Î²-Hairpin Fold from Its Transition State?. Journal of Physical Chemistry B, 2014, 118, 3317-3325.	2.7	15
34	Stable Saltâ€“Water Cluster Structures Reflect the Delicate Competition between Ionâ€“Water and Waterâ€“Water Interactions. Journal of Physical Chemistry B, 2014, 118, 743-751.	2.7	43
35	Dynamics of spontaneous flipping of a mismatched base in DNA duplex. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 8043-8048.	7.5	83
36	Modeling the Thermal Unfolding 2DIR Spectra of a Î²-Hairpin Peptide Based on the Implicit Solvent MD Simulation. Journal of Physical Chemistry A, 2013, 117, 6256-6263.	2.6	6

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37	From protein denaturant to protectant: Comparative molecular dynamics study of alcohol/protein interactions. Journal of Chemical Physics, 2012, 136, 115101.	3.0	44
38	Counterion Effects on the Denaturing Activity of Guanidinium Cation to Protein. Journal of Chemical Theory and Computation, 2012, 8, 4364-4373.	5.5	13
39	Differences of Cations and Anions: Their Hydration, Surface Adsorption, and Impact on Water Dynamics. Journal of Physical Chemistry B, 2011, 115, 12456-12465.	2.7	70
40	Structure change of Î²-hairpin induced by turn optimization: An enhanced sampling molecular dynamics simulation study. Journal of Chemical Physics, 2011, 135, 235104.	3.0	21
41	Effects of Cosolvents on the Hydration of Carbon Nanotubes. Journal of the American Chemical Society, 2010, 132, 842-848.	14.5	50
42	Mutation of Charged Residues to Neutral Ones Accelerates Urea Denaturation of HP-35. Journal of Physical Chemistry B, 2010, 114, 11820-11826.	2.7	20
43	Comparison between integrated and parallel tempering methods in enhanced sampling simulations. Journal of Chemical Physics, 2009, 130, 124111.	3.0	44
44	A selective integrated tempering method. Journal of Chemical Physics, 2009, 131, 214109.	3.0	57
45	A test of implicit solvent models on the folding simulation of the GB1 peptide. Journal of Chemical Physics, 2009, 130, 195104.	3.0	23
46	On the Structure of Water at the Aqueous/Air Interface. Journal of Physical Chemistry B, 2009, 113, 11672-11679.	2.7	134
47	Thermodynamics and Folding Pathways of Trpzip2: An Accelerated Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2009, 113, 803-808.	2.7	56
48	Thermodynamics and kinetics simulations of multi-time-scale processes for complex systems. International Reviews in Physical Chemistry, 2008, 27, 201-227.	1.9	41
49	Selective sampling of transition paths. Journal of Chemical Physics, 2007, 127, 154106.	3.0	18
50	An Approximate Method in Using Molecular Mechanics Simulations To Study Slow Protein Conformational Changes. Journal of Physical Chemistry B, 2007, 111, 2969-2975.	2.7	9
51	Application of the accelerated molecular dynamics simulations to the folding of a small protein. Journal of Chemical Physics, 2007, 126, 125102.	3.0	38