Pratyush Tiwary

List of Publications by Year
in descending order

Version: 2024-02-01

53 papers	4,076 citations	212478 28 h-index	223390 49 g-index
62 all docs	62 docs citations	62 times ranked	3314 citing authors

#	Article	IF	Citations
1	Influence of Long-Range Forces on the Transition States and Dynamics of NaCl Ion-Pair Dissociation in Water. Journal of Physical Chemistry B, 2022, 126, 545-551.	1.2	5
2	Accelerating All-Atom Simulations and Gaining Mechanistic Understanding of Biophysical Systems through State Predictive Information Bottleneck. Journal of Chemical Theory and Computation, 2022, 18, 3231-3238.	2.3	21
3	Protein Flexibility and Dissociation Pathway Differentiation Can Explain Onset of Resistance Mutations in Kinases**. Angewandte Chemie - International Edition, 2022, 61, e202200983.	7.2	21
4	Interrogating RNAâ€“Small Molecule Interactions with Structure Probing and Artificial Intelligence-Augmented Molecular Simulations. ACS Central Science, 2022, 8, 741-748.	5.3	15
5	Quantifying Energetic and Entropic Pathways in Molecular Systems. Journal of Physical Chemistry B, 2022, 126, 3950-3960.	1.2	5
6	On the distance between A and B in molecular configuration space. Molecular Simulation, 2021, 47, 449-456.	0.9	4
7	Editorial: Molecular Dynamics and Machine Learning in Drug Discovery. Frontiers in Molecular Biosciences, 2021, 8, 673773.	1.6	8
8	State predictive information bottleneck. Journal of Chemical Physics, 2021, 154, 134111.	1.2	51
9	Making High-Dimensional Molecular Distribution Functions Tractable through Belief Propagation on Factor Graphs. Journal of Physical Chemistry B, 2021, 125, 11150-11158.	1.2	0
10	SGOOP-d: Estimating Kinetic Distances and Reaction Coordinate Dimensionality for Rare Event Systems from Biased/Unbiased Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6757-6765.	2.3	25
11	Toward Automated Sampling of Polymorph Nucleation and Free Energies with the SGOOP and Metadynamics. Journal of Physical Chemistry B, 2021, 125, 13049-13056.	1.2	9
12	Automatic mutual information noise omission (AMINO): generating order parameters for molecular systems. Molecular Systems Design and Engineering, 2020, 5, 339-348.	1.7	39
13	Learning molecular dynamics with simple language model built upon long short-term memory neural network. Nature Communications, 2020, 11, 5115.	5.8	52
14	Discovering Protein Conformational Flexibility through Artificial-Intelligence-Aided Molecular Dynamics. Journal of Physical Chemistry B, 2020, 124, 8221-8229.	1.2	22
15	Machine learning approaches for analyzing and enhancing molecular dynamics simulations. Current Opinion in Structural Biology, 2020, 61, 139-145.	2.6	176
16	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2020, , 565-595.		13
17	Understanding the role of predictive time delay and biased propagator in RAVE. Journal of Chemical Physics, 2020, 152, 144102.	1.2	11
18	Confronting pitfalls of AI-augmented molecular dynamics using statistical physics. Journal of Chemical Physics, 2020, 153, 234118.	1.2	12

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19	Pastâ€“future information bottleneck for sampling molecular reaction coordinate simultaneously with thermodynamics and kinetics. Nature Communications, 2019, 10, 3573.	5.8	102
20	Reaction coordinates and rate constants for liquid droplet nucleation: Quantifying the interplay between driving force and memory. Journal of Chemical Physics, 2019, 151, 154106.	1.2	18
21	Can One Trust Kinetic and Thermodynamic Observables from Biased Metadynamics Simulations?: Detailed Quantitative Benchmarks on Millimolar Drug Fragment Dissociation. Journal of Physical Chemistry B, 2019, 123, 3672-3678.	1.2	34
22	Toward Achieving Efficient and Accurate Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE. Journal of Chemical Theory and Computation, 2019, 15, 708-719.	2.3	61
23	Kinetics of Ligandâ€“Protein Dissociation from All-Atom Simulations: Are We There Yet?. Biochemistry, 2019, 58, 156-165.	1.2	35
24	Metadynamics: A Unified Framework for Accelerating Rare Events and Sampling Thermodynamics and Kinetics. , 2018, , 1-31.		11
25	Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional probability factorization. Journal of Chemical Physics, 2018, 149, 234105.	1.2	34
26	Frequency adaptive metadynamics for the calculation of rare-event kinetics. Journal of Chemical Physics, 2018, 149, 072309.	1.2	54
27	Reweighted autoencoded variational Bayes for enhanced sampling (RAVE). Journal of Chemical Physics, 2018, 149, 072301.	1.2	219
28	How and when does an anticancer drug leave its binding site?. Science Advances, 2017, 3, e1700014.	4.7	111
29	Predicting reaction coordinates in energy landscapes with diffusion anisotropy. Journal of Chemical Physics, 2017, 147, 152701.	1.2	37
30	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. Journal of the American Chemical Society, 2017, 139, 4780-4788.	6.6	187
31	Molecular Determinants and Bottlenecks in the Dissociation Dynamics of Biotinâ€“Streptavidin. Journal of Physical Chemistry B, 2017, 121, 10841-10849.	1.2	32
32	Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review. Current Topics in Medicinal Chemistry, 2017, 17, 2626-2641.	1.0	44
33	How wet should be the reaction coordinate for ligand unbinding?. Journal of Chemical Physics, 2016, 145, 054113.	1.2	31
34	Kramers turnover: From energy diffusion to spatial diffusion using metadynamics. Journal of Chemical Physics, 2016, 144, 134103.	1.2	18
35	Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations. Journal of Chemical Physics, 2016, 145, 211925.	1.2	40
36	Prediction of Proteinâ€“Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 2990-2998.	2.3	184

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37	A Review of Enhanced Sampling Approaches for Accelerated Molecular Dynamics. Springer Series in Materials Science, 2016, , 195-221.	0.4	60
38	Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint. Annual Review of Physical Chemistry, 2016, 67, 159-184.	4.8	497
39	Spectral gap optimization of order parameters for sampling complex molecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2839-2844.	3.3	210
40	How a Kinase Inhibitor Withstands Gatekeeper Residue Mutations. Journal of the American Chemical Society, 2016, 138, 4608-4615.	6.6	44
41	New Approach for Investigating Reaction Dynamics and Rates with Ab Initio Calculations. Journal of Physical Chemistry A, 2016, 120, 299-305.	1.1	44
42	Variationally Optimized Free-Energy Flooding for Rate Calculation. Physical Review Letters, 2015, 115, 070601.	2.9	35
43	A perturbative solution to metadynamics ordinary differential equation. Journal of Chemical Physics, 2015, 143, 234112.	1.2	13
44	Path Integral Metadynamics. Journal of Chemical Theory and Computation, 2015, 11, 1383-1388.	2.3	21
45	Kinetics of proteinâ€“ligand unbinding: Predicting pathways, rates, and rate-limiting steps. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E386-91.	3.3	311
46	de Broglie Swapping Metadynamics for Quantum and Classical Sampling. Journal of Chemical Theory and Computation, 2015, 11, 5114-5119.	2.3	9
47	Role of water and steric constraints in the kinetics of cavityâ€“ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019.	3.3	74
48	A Time-Independent Free Energy Estimator for Metadynamics. Journal of Physical Chemistry B, 2015, 119, 736-742.	1.2	399
49	Assessing the Reliability of the Dynamics Reconstructed from Metadynamics. Journal of Chemical Theory and Computation, 2014, 10, 1420-1425.	2.3	175
50	From Metadynamics to Dynamics. Physical Review Letters, 2013, 111, 230602.	2.9	369
51	Accelerated molecular dynamics through stochastic iterations and collective variable based basin identification. Physical Review B, 2013, 87, .	1.1	31
52	Hybrid deterministic and stochastic approach for efficient atomistic simulations at long time scales. Physical Review B, 2011, 84, .	1.1	26
53	Protein Flexibility and Dissociation Pathway Differentiation Can Explain Onset Of Resistance Mutations in Kinases. Angewandte Chemie, 0, , .	1.6	0