Tristan Bereau

List of Publications by Year
in descending order

72 papers	1,872 citations	304602 22 h-index	289141 40 g-index
77 all docs	77 docs citations	77 times ranked	1877 citing authors

#	Article	IF	Citations
1	Data-driven discovery of cardiolipin-selective small molecules by computational active learning. Chemical Science, 2022, 13, 4498-4511.	3.7	18
2	FAIR data enabling new horizons for materials research. Nature, 2022, 604, 635-642.	13.7	81
3	Computational compound screening of biomolecules and soft materials by molecular simulations. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 023001.	0.8	15
4	The Bacteriostatic Activity of 2-Phenylethanol Derivatives Correlates with Membrane Binding Affinity. Membranes, 2021, 11, 254.	1.4	12
5	Adversarial reverse mapping of condensed-phase molecular structures: Chemical transferability. APL Materials, 2021, 9, .	2.2	17
6	Reweighting non-equilibrium steady-state dynamics along collective variables. Journal of Chemical Physics, 2021, 154, 134105.	1.2	2
7	Dynamical properties across different coarse-grained models for ionic liquids. Journal of Physics Condensed Matter, 2021, 33, 224001.	0.7	7
8	Computer simulations of lipid regulation by molecular semigrand canonical ensembles. Biophysical Journal, 2021, 120, 2370-2373.	0.2	1
9	Finite-size transitions in complex membranes. Biophysical Journal, 2021, 120, 2436-2443.	0.2	3
10	Data-driven equation for drugâ€“membrane permeability across drugs and membranes. Journal of Chemical Physics, 2021, 154, 244114.	1.2	13
11	Multipolar Force Fields for Amide-I Spectroscopy from Conformational Dynamics of the Alanine Trimer. Journal of Physical Chemistry B, 2021, 125, 10928-10938.	1.2	6
12	Regulating Lipid Composition Rationalizes Acyl Tail Saturation Homeostasis in Ectotherms. Biophysical Journal, 2020, 119, 892-899.	0.2	10
13	Coarse-grained conformational surface hopping: Methodology and transferability. Journal of Chemical Physics, 2020, 153, 214110.	1.2	14
14	Hydration free energies from kernel-based machine learning: Compound-database bias. Journal of Chemical Physics, 2020, 153, 014101.	1.2	23
15	Free-energy landscape of polymer-crystal polymorphism. Soft Matter, 2020, 16, 9683-9692.	1.2	9
16	Designing exceptional gas-separation polymer membranes using machine learning. Science Advances, 2020, 6, eaaz4301.	4.7	132
17	Interpretable embeddings from molecular simulations using Gaussian mixture variational autoencoders. Machine Learning: Science and Technology, 2020, 1, 015012.	2.4	26
18	Inserting Small Molecules across Membrane Mixtures: Insight from the Potential of Mean Force. Biophysical Journal, 2020, 118, 1321-1332.	0.2	15

#	Article	IF	Citations
19	Molecular dynamics trajectories for 630 coarse-grained drug-membrane permeations. Scientific Data, 2020, 7, 51.	2.4	23
20	Probing Nanoparticle/Membrane Interactions by Combining Amphiphilic Diblock Copolymer Assembly and Plasmonics. Journal of Physical Chemistry B, 2020, 124, 742-750.	1.2	7
21	Kernel-Based Machine Learning for Efficient Simulations of Molecular Liquids. Journal of Chemical Theory and Computation, 2020, 16, 3194-3204.	2.3	44
22	Adversarial reverse mapping of equilibrated condensed-phase molecular structures. Machine Learning: Science and Technology, 2020, 1, 045014.	2.4	23
23	Data-Driven Methods in Multiscale Modeling of Soft Matter. , 2020, , 1459-1470.		2
24	Resolution limit of data-driven coarse-grained models spanning chemical space. Journal of Chemical Physics, 2019, 151, 164106.	1.2	22
25	Controlled exploration of chemical space by machine learning of coarse-grained representations. Physical Review E, 2019, 100, 033302.	0.8	17
26	Hoobas: A highly object-oriented builder for molecular dynamics. Computational Materials Science, 2019, 167, 25-33.	1.4	20
27	Revisiting the Meyer-Overton rule for drug-membrane permeabilities. Molecular Physics, 2019, 117, 2900-2909.	0.8	10
28	Conformationally-Dependent Surface Hopping for Reproducing Structural Cross-Correlations with Coarse-Grained Models. Biophysical Journal, 2019, 116, 304a.	0.2	0
29	Investigating Drug-Membrane Permeability across Chemical Compound Space using High-Throughput Coarse-Grained Simulations. Biophysical Journal, 2019, 116, 318a.	0.2	1
30	Sequenceâ€Optimized Peptide Nanofibers as Growth Stimulators for Regeneration of Peripheral Neurons. Advanced Functional Materials, 2019, 29, 1809112.	7.8	19
31	Direct route to reproducing pair distribution functions with coarse-grained models via transformed atomistic cross correlations. Journal of Chemical Physics, 2019, 151, 244110.	1.2	8
32	Microscopic reweighting for nonequilibrium steady-state dynamics. Physical Review E, 2019, 100, 060103.	0.8	5
33	Drugâ€“Membrane Permeability across Chemical Space. ACS Central Science, 2019, 5, 290-298.	5.3	67
34	Automated detection of many-particle solvation states for accurate characterizations of diffusion kinetics. Journal of Chemical Physics, 2019, 150, 024102.	1.2	3
35	Engineering Proteins at Interfaces: From Complementary Characterization to Material Surfaces with Designed Functions. Angewandte Chemie - International Edition, 2018, 57, 12626-12648.	7.2	40
36	Engineering von Proteinen an OberflÃchen: Von komplementÃrer Charakterisierung zu MaterialoberflÃchen mit maÃŸgeschneiderten Funktionen. Angewandte Chemie, 2018, 130, 12806-12830.	1.6	3

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37	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. Journal of Chemical Physics, 2018, 148, 241706.	1.2	136
38	Efficient potential of mean force calculation from multiscale simulations: Solute insertion in a lipid membrane. Biochemical and Biophysical Research Communications, 2018, 498, 282-287.	1.0	20
39	Accurate Structure-Based Coarse Graining Leads to Consistent Barrier-Crossing Dynamics. Physical Review Letters, 2018, 121, 256002.	2.9	24
40	Polymorphism of Syndiotactic Polystyrene Crystals from Multiscale Simulations. Advanced Theory and Simulations, 2018, 1, 1800024.	1.3	16
41	The Role of Conformational Entropy in the Determination of Structural-Kinetic Relationships for Helix-Coil Transitions. Computation, 2018, 6, 21.	1.0	9
42	Data-Driven Methods in Multiscale Modeling of Soft Matter. , 2018, , 1-12.		0
43	Structural-kinetic-thermodynamic relationships identified from physics-based molecular simulation models. Journal of Chemical Physics, 2018, 148, 204111.	1.2	7
44	Nitrated Fatty Acids Modulate the Physical Properties of Model Membranes and the Structure of Transmembrane Proteins. Chemistry - A European Journal, 2017, 23, 9690-9697.	1.7	17
45	In silico screening of drug-membrane thermodynamics reveals linear relations between bulk partitioning and the potential of mean force. Journal of Chemical Physics, 2017, 147, 125101.	1.2	37
46	Research Update: Computational materials discovery in soft matter. APL Materials, 2016, 4, .	2.2	34
47	Communication: Consistent interpretation of molecular simulation kinetics using Markov state models biased with external information. Journal of Chemical Physics, 2016, 144, 051102.	1.2	31
48	Impact of Quadrupolar Electrostatics on Atoms Adjacent to the Sigma-Hole in Condensed-Phase Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3008-3019.	2.3	23
49	Concurrent parametrization against static and kinetic information leads to more robust coarse-grained force fields. European Physical Journal: Special Topics, 2016, 225, 1373-1389.	1.2	17
50	Protein-Backbone Thermodynamics across the Membrane Interface. Journal of Physical Chemistry B, 2016, 120, 6391-6400.	1.2	6
51	An in-silico walker. Chemical Physics Letters, 2016, 659, 6-9.	1.2	2
52	Folding and insertion thermodynamics of the transmembrane WALP peptide. Journal of Chemical Physics, 2015, 143, 243127.	1.2	37
53	Transferable Atomic Multipole Machine Learning Models for Small Organic Molecules. Journal of Chemical Theory and Computation, 2015, 11, 3225-3233.	2.3	91
54	Better Together: Lipopeptide Micelle Formation Enhances Antimicrobial Selectivity. Biophysical Journal, 2015, 109, 668-669.	0.2	2

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55	Multipolar Force Fields and Their Effects on Solvent Dynamics around Simple Solutes. Journal of Physical Chemistry B, 2015, 119, 3034-3045.	1.2	10
56	Automated Parametrization of the Coarse-Grained Martini Force Field for Small Organic Molecules. Journal of Chemical Theory and Computation, 2015, 11, 2783-2791.	2.3	117
57	Solvation of fluoro-acetonitrile in water by 2D-IR spectroscopy: A combined experimental-computational study. Journal of Chemical Physics, 2015, 142, 212415.	1.2	13
58	Multi-timestep Integrator for the Modified Andersen Barostat. Physics Procedia, 2015, 68, 7-15.	1.2	3
59	Enhanced Sampling of Coarse-Grained Transmembrane-Peptide Structure Formation from Hydrogen-Bond Replica Exchange. Journal of Membrane Biology, 2015, 248, 395-405.	1.0	12
60	More than the sum of its parts: Coarse-grained peptide-lipid interactions from a simple cross-parametrization. Journal of Chemical Physics, 2014, 140, 115101.	1.2	38
61	Toward transferable interatomic van der Waals interactions without electrons: The role of multipole electrostatics and many-body dispersion. Journal of Chemical Physics, 2014, 141, 034101.	1.2	17
62	Computational Two-Dimensional Infrared Spectroscopy without Maps: N-Methylacetamide in Water. Journal of Physical Chemistry B, 2014, 118, 8135-8147.	1.2	27
63	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	2.5	25
64	Scoring Multipole Electrostatics in Condensed-Phase Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 5460-5471.	1.2	18
65	Leveraging Symmetries of Static Atomic Multipole Electrostatics in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 5450-5459.	2.3	49
66	Coarse-Grained and Atomistic Simulations of the Salt-Stable Cowpea Chlorotic Mottle Virus (SS-CCMV) Subunit 26â€“49: Î²-Barrel Stability of the Hexamer and Pentamer Geometries. Journal of Chemical Theory and Computation, 2012, 8, 3750-3758.	2.3	22
67	Structural Basis of Folding Cooperativity in Model Proteins: Insights from a Microcanonical Perspective. Biophysical Journal, 2011, 100, 2764-2772.	0.2	32
68	Identifying Two-State Transitions by Microcanonical Analysis: Coarse-Grained Simulations of Helical Peptides. Biophysical Journal, 2010, 98, 634a.	0.2	0
69	Interplay between Secondary and Tertiary Structure Formation in Protein Folding Cooperativity. Journal of the American Chemical Society, 2010, 132, 13129-13131.	6.6	48
70	Optimized convergence for multiple histogram analysis. Journal of Computational Physics, 2009, 228, 6119-6129.	1.9	29
71	Generic coarse-grained model for protein folding and aggregation. Journal of Chemical Physics, 2009, 130, 235106.	1.2	182
72	CLiB â€“ a novel cardiolipin-binder isolated via data-driven and in vitro screening. RSC Chemical Biology, 0, , .	2.0	1