Frank No

List of Publications by Citations

151 papers	10,303 citations	51 h-index	99 g-index
170 ext. papers	13,227 ext. citations	7.8 avg, IF	7.09 L-index

#	Paper	IF	Citations
151	Markov models of molecular kinetics: generation and validation. *Journal of Chemical Physics*, **2011**, 134, 174105	3.9	738
150	Constructing the equilibrium ensemble of folding pathways from short off-equilibrium simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 19011-6	11.5	586
149	Identification of slow molecular order parameters for Markov model construction. *Journal of Chemical Physics*, **2013**, 139, 015102	3.9	522
148	PyEMMA 2: A Software Package for Estimation, Validation, and Analysis of Markov Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 5525-42	6.4	504
147	Markov state models of biomolecular conformational dynamics. *Current Opinion in Structural Biology*, **2014**, 25, 135-44	8.1	448
146	Hierarchical analysis of conformational dynamics in biomolecules: transition networks of metastable states. *Journal of Chemical Physics*, **2007**, 126, 155102	3.9	322
145	Spatiotemporal control of endocytosis by phosphatidylinositol-3,4-bisphosphate. *Nature*, **2013**, 499, 233-7	50.4	289
144	Protein conformational plasticity and complex ligand-binding kinetics explored by atomistic simulations and Markov models. *Nature Communications*, **2015**, 6, 7653	17.4	252
143	Crystal structure of nucleotide-free dynamin. *Nature*, **2011**, 477, 556-60	50.4	229
142	HTMD: High-Throughput Molecular Dynamics for Molecular Discovery. *Journal of Chemical Theory and Computation*, **2016**, 12, 1845-52	6.4	219
141	Complete protein-protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling. *Nature Chemistry*, **2017**, 9, 1005-1011	17.6	203
140	Machine Learning for Molecular Simulation. *Annual Review of Physical Chemistry*, **2020**, 71, 361-390	15.7	193
139	Variational Approach to Molecular Kinetics. *Journal of Chemical Theory and Computation*, **2014**, 10, 1739-52	6.4	193
138	A Variational Approach to Modeling Slow Processes in Stochastic Dynamical Systems. *Multiscale Modeling and Simulation*, **2013**, 11, 635-655	1.8	180
137	VAMPnets for deep learning of molecular kinetics. *Nature Communications*, **2018**, 9, 5	17.4	168
136	Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning. *Science*, **2019**, 365,	33.3	166
135	Markov state models based on milestoning. *Journal of Chemical Physics*, **2011**, 134, 204105	3.9	164

134	Time-lagged autoencoders: Deep learning of slow collective variables for molecular kinetics. *Journal of Chemical Physics*, **2018**, 148, 241703	3.9	162
133	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. *ACS Central Science*, **2019**, 5, 755-767	7.8	160
132	On the Approximation Quality of Markov State Models. *Multiscale Modeling and Simulation*, **2010**, 8, 1154-8177	1.8	153
131	Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. *Chemical Science*, **2019**, 10, 1692-1701	9.4	152
130	Multiensemble Markov models of molecular thermodynamics and kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E3221-30	11.5	133
129	Data-Driven Model Reduction and Transfer Operator Approximation. *Journal of Nonlinear Science*, **2018**, 28, 985-1010	2.8	124
128	EMMA: A Software Package for Markov Model Building and Analysis. *Journal of Chemical Theory and Computation*, **2012**, 8, 2223-38	6.4	123
127	Camostat mesylate inhibits SARS-CoV-2 activation by TMPRSS2-related proteases and its metabolite GBPA exerts antiviral activity. *EBioMedicine*, **2021**, 65, 103255	8.8	120
126	Kinetic distance and kinetic maps from molecular dynamics simulation. *Journal of Chemical Theory and Computation*, **2015**, 11, 5002-11	6.4	113
125	Probability distributions of molecular observables computed from Markov models. *Journal of Chemical Physics*, **2008**, 128, 244103	3.9	110
124	Deep-neural-network solution of the electronic Schrödinger equation. *Nature Chemistry*, **2020**, 12, 891-897	17.6	103
123	Projected and hidden Markov models for calculating kinetics and metastable states of complex molecules. *Journal of Chemical Physics*, **2013**, 139, 184114	3.9	96
122	ReaDDy--a software for particle-based reaction-diffusion dynamics in crowded cellular environments. *PLoS ONE*, **2013**, 8, e74261	3.7	91
121	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 4822-7	11.5	90
120	Higher-order architecture of rhodopsin in intact photoreceptors and its implication for phototransduction kinetics. *Structure*, **2015**, 23, 628-38	5.2	89
119	Probing molecular kinetics with Markov models: metastable states, transition pathways and spectroscopic observables. *Physical Chemistry Chemical Physics*, **2011**, 13, 16912-27	3.6	86
118	Kinetic characterization of the critical step in HIV-1 protease maturation. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 20449-54	11.5	85
117	Crystal structure of the dynamin tetramer. *Nature*, **2015**, 525, 404-8	50.4	82

116	Transition Networks for the Comprehensive Characterization of Complex Conformational Change in Proteins. *Journal of Chemical Theory and Computation*, **2006**, 2, 840-57	6.4	81
115	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. *Nature Communications*, **2017**, 8, 1095	17.4	76
114	Nanoscopic compartmentalization of membrane protein motion at the axon initial segment. *Journal of Cell Biology*, **2016**, 215, 37-46	7.3	71
113	Collective variables for the study of long-time kinetics from molecular trajectories: theory and methods. *Current Opinion in Structural Biology*, **2017**, 43, 141-147	8.1	69
112	Complex RNA folding kinetics revealed by single-molecule FRET and hidden Markov models. *Journal of the American Chemical Society*, **2014**, 136, 4534-43	16.4	69
111	Estimation and uncertainty of reversible Markov models. *Journal of Chemical Physics*, **2015**, 143, 174101	3.9	67
110	Lipid-mediated PX-BAR domain recruitment couples local membrane constriction to endocytic vesicle fission. *Nature Communications*, **2017**, 8, 15873	17.4	66
109	Variational Approach for Learning Markov Processes from Time Series Data. *Journal of Nonlinear Science*, **2020**, 30, 23-66	2.8	66
108	Efficient multi-objective molecular optimization in a continuous latent space. *Chemical Science*, **2019**, 10, 8016-8024	9.4	63
107	Combining experimental and simulation data of molecular processes via augmented Markov models. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 8265-8270	11.5	62
106	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. *Journal of Chemical Physics*, **2014**, 141, 214106	3.9	62
105	Dynamic properties of force fields. *Journal of Chemical Physics*, **2015**, 142, 084101	3.9	60
104	Variational Koopman models: Slow collective variables and molecular kinetics from short off-equilibrium simulations. *Journal of Chemical Physics*, **2017**, 146, 154104	3.9	58
103	Simulation tools for particle-based reaction-diffusion dynamics in continuous space. *BMC Biophysics* , **2014**, 7, 11	0	56
102	Machine learning for protein folding and dynamics. *Current Opinion in Structural Biology*, **2020**, 60, 77-84	8.1	55
101	Mechanisms of protein-ligand association and its modulation by protein mutations. *Biophysical Journal*, **2011**, 100, 701-710	2.9	54
100	Structure and assembly of the mitochondrial membrane remodelling GTPase Mgm1. *Nature*, **2019**, 571, 429-433	50.4	50
99	Dynamical reweighting: improved estimates of dynamical properties from simulations at multiple temperatures. *Journal of Chemical Physics*, **2011**, 134, 244107	3.9	50

98	Markov models and dynamical fingerprints: Unraveling the complexity of molecular kinetics. *Chemical Physics*, **2012**, 396, 92-107	2.3	48
97	Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. *Journal of Chemical Physics*, **2011**, 134, 244108	3.9	43
96	Variational tensor approach for approximating the rare-event kinetics of macromolecular systems. *Journal of Chemical Physics*, **2016**, 144, 054105	3.9	43
95	Hierarchical Time-Lagged Independent Component Analysis: Computing Slow Modes and Reaction Coordinates for Large Molecular Systems. *Journal of Chemical Theory and Computation*, **2016**, 12, 6118-6129	6.4	41
94	Commute Maps: Separating Slowly Mixing Molecular Configurations for Kinetic Modeling. *Journal of Chemical Theory and Computation*, **2016**, 12, 5620-5630	6.4	40
93	Investigating Molecular Kinetics by Variationally Optimized Diffusion Maps. *Journal of Chemical Theory and Computation*, **2015**, 11, 5947-60	6.4	39
92	Dynamical Organization of Syntaxin-1A at the Presynaptic Active Zone. *PLoS Computational Biology*, **2015**, 11, e1004407	5	38
91	Markov state models from short non-equilibrium simulations—Analysis and correction of estimation bias. *Journal of Chemical Physics*, **2017**, 146, 094104	3.9	37
90	Estimating the sampling error: distribution of transition matrices and functions of transition matrices for given trajectory data. *Physical Review E*, **2009**, 80, 021106	2.4	36
89	Alpha 1 Antitrypsin is an Inhibitor of the SARS-CoV-2-Priming Protease TMPRSS2. *Pathogens and Immunity*, **2021**, 6, 55-74	4.9	36
88	Coarse graining molecular dynamics with graph neural networks. *Journal of Chemical Physics*, **2020**, 153, 194101	3.9	34
87	Unsupervised Learning Methods for Molecular Simulation Data. *Chemical Reviews*, **2021**, 121, 9722-9758	68.1	34
86	Data-based parameter estimation of generalized multidimensional Langevin processes. *Physical Review E*, **2007**, 76, 016706	2.4	33
85	Explicit spatiotemporal simulation of receptor-G protein coupling in rod cell disk membranes. *Biophysical Journal*, **2014**, 107, 1042-1053	2.9	32
84	Probability distributions of molecular observables computed from Markov models. II. Uncertainties in observables and their time-evolution. *Journal of Chemical Physics*, **2010**, 133, 105102	3.9	32
83	Automated computation of low-energy pathways for complex rearrangements in proteins: application to the conformational switch of Ras p21. *Proteins: Structure, Function and Bioinformatics* , **2005**, 59, 534-44	4.2	32
82	Camostat mesylate inhibits SARS-CoV-2 activation by TMPRSS2-related proteases and its metabolite GBPA exerts antiviral activity **2020**,		30
81	Reactive SINDy: Discovering governing reactions from concentration data. *Journal of Chemical Physics*, **2019**, 150, 025101	3.9	29

80	MHC class II complexes sample intermediate states along the peptide exchange pathway. *Nature Communications*, **2016**, 7, 13224	17.4	29
79	Efficient Bayesian estimation of Markov model transition matrices with given stationary distribution. *Journal of Chemical Physics*, **2013**, 138, 164113	3.9	29
78	Shedding Light on the Dock-Lock Mechanism in Amyloid Fibril Growth Using Markov State Models. *Journal of Physical Chemistry Letters*, **2015**, 6, 1076-81	6.4	28
77	Introduction to Markov state modeling with the PyEMMA software [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1,	10.1	28
76	It takes two transducins to activate the cGMP-phosphodiesterase 6 in retinal rods. *Open Biology*, **2018**, 8,	7	28
75	ReaDDy 2: Fast and flexible software framework for interacting-particle reaction dynamics. *PLoS Computational Biology*, **2019**, 15, e1006830	5	27
74	OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics. *Journal of Chemical Theory and Computation*, **2019**, 15, 813-836	6.4	27
73	Molecular mechanism of inhibiting the SARS-CoV-2 cell entry facilitator TMPRSS2 with camostat and nafamostat.. *Chemical Science*, **2021**, 12, 983-992	9.4	27
72	Variational selection of features for molecular kinetics. *Journal of Chemical Physics*, **2019**, 150, 194108	3.9	25
71	Ensemble learning of coarse-grained molecular dynamics force fields with a kernel approach. *Journal of Chemical Physics*, **2020**, 152, 194106	3.9	25
70	ReaDDyMM: Fast interacting particle reaction-diffusion simulations using graphical processing units. *Biophysical Journal*, **2015**, 108, 457-61	2.9	25
69	Alpha 1 Antitrypsin is an Inhibitor of the SARS-CoV-2-Priming Protease TMPRSS2 **2020**,		24
68	A Basis Set for Peptides for the Variational Approach to Conformational Kinetics. *Journal of Chemical Theory and Computation*, **2015**, 11, 3992-4004	6.4	23
67	xTRAM: Estimating Equilibrium Expectations from Time-Correlated Simulation Data at Multiple Thermodynamic States. *Physical Review X*, **2014**, 4,	9.1	23
66	TorchMD: A Deep Learning Framework for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 2355-2363	6.4	23
65	Targeted Adversarial Learning Optimized Sampling. *Journal of Physical Chemistry Letters*, **2019**, 10, 5791-5797	6.4	22
64	Dynamically Driven Allostery in MHC Proteins: Peptide-Dependent Tuning of Class I MHC Global Flexibility. *Frontiers in Immunology*, **2019**, 10, 966	8.4	22
63	Predicting the Kinetics of RNA Oligonucleotides Using Markov State Models. *Journal of Chemical Theory and Computation*, **2017**, 13, 926-934	6.4	21

62	Optimal Estimation of Free Energies and Stationary Densities from Multiple Biased Simulations. *Multiscale Modeling and Simulation*, **2014**, 12, 25-54	1.8	21
61	Dynamic neutron scattering from conformational dynamics. I. Theory and Markov models. *Journal of Chemical Physics*, **2013**, 139, 175101	3.9	20
60	Single event visualization of unconventional secretion of FGF2. *Journal of Cell Biology*, **2019**, 218, 683-699	7.3	20
59	OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes. *Journal of Chemical Theory and Computation*, **2019**, 15, 837-856	6.4	20
58	The Isomeric Preference of an Atypical Dopamine Transporter Inhibitor Contributes to Its Selection of the Transporter Conformation. *ACS Chemical Neuroscience*, **2017**, 8, 1735-1746	5.7	18
57	Mechanistic Models of Chemical Exchange Induced Relaxation in Protein NMR. *Journal of the American Chemical Society*, **2017**, 139, 200-210	16.4	18
56	Optimal identification of semi-rigid domains in macromolecules from molecular dynamics simulation. *PLoS ONE*, **2010**, 5, e10491	3.7	18
55	MSM/RD: Coupling Markov state models of molecular kinetics with reaction-diffusion simulations. *Journal of Chemical Physics*, **2018**, 148, 214107	3.9	17
54	Beating the millisecond barrier in molecular dynamics simulations. *Biophysical Journal*, **2015**, 108, 228-9	2.9	16
53	Optimal Data-Driven Estimation of Generalized Markov State Models for Non-Equilibrium Dynamics. *Computation*, **2018**, 6, 22	2.2	16
52	Dynamic graphical models of molecular kinetics. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 15001-15006	11.5	16
51	Reversible Interacting-Particle Reaction Dynamics. *Journal of Physical Chemistry B*, **2018**, 122, 11240-11250	3.4	16
50	Identification of kinetic order parameters for non-equilibrium dynamics. *Journal of Chemical Physics* , **2019**, 150, 164120	3.9	15
49	Particle-based membrane model for mesoscopic simulation of cellular dynamics. *Journal of Chemical Physics*, **2018**, 148, 044901	3.9	15
48	Identifying Conformational-Selection and Induced-Fit Aspects in the Binding-Induced Folding of PMI from Markov State Modeling of Atomistic Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 5649-5656	3.4	15
47	Spectral Rate Theory for Two-State Kinetics. *Physical Review X*, **2014**, 4,	9.1	15
46	An efficient multi-scale Green's function reaction dynamics scheme. *Journal of Chemical Physics*, **2017**, 147, 184106	3.9	14
45	Collective hydrogen-bond rearrangement dynamics in liquid water. *Journal of Chemical Physics*, **2018**, 149, 244504	3.9	14

44	Gaussian Markov transition models of molecular kinetics. *Journal of Chemical Physics*, **2015**, 142, 084104	3.9	13
43	The mechanism of RNA base fraying: Molecular dynamics simulations analyzed with core-set Markov state models. *Journal of Chemical Physics*, **2019**, 150, 154123	3.9	12
42	Large-scale simulation of biomembranes incorporating realistic kinetics into coarse-grained models. *Nature Communications*, **2020**, 11, 2951	17.4	12
41	Diffusion-influenced reaction rates in the presence of pair interactions. *Journal of Chemical Physics*, **2019**, 151, 164105	3.9	12
40	Projected metastable Markov processes and their estimation with observable operator models. *Journal of Chemical Physics*, **2015**, 143, 144101	3.9	12
39	Dynamic neutron scattering from conformational dynamics. II. Application using molecular dynamics simulation and Markov modeling. *Journal of Chemical Physics*, **2013**, 139, 175102	3.9	11
38	Neuraldecipher - reverse-engineering extended-connectivity fingerprints (ECFPs) to their molecular structures. *Chemical Science*, **2020**, 11, 10378-10389	9.4	11
37	Rapid Calculation of Molecular Kinetics Using Compressed Sensing. *Journal of Chemical Theory and Computation*, **2018**, 14, 2771-2783	6.4	10
36	Molecular dynamics simulations data of the twenty encoded amino acids in different force fields. *Data in Brief*, **2016**, 7, 582-90	1.2	10
35	Machine Learning for Molecular Dynamics on Long Timescales. *Lecture Notes in Physics*, **2020**, 331-372	0.8	10
34	What Markov State Models Can and Cannot Do: Correlation versus Path-Based Observables in Protein-Folding Models. *Journal of Chemical Theory and Computation*, **2021**, 17, 3119-3133	6.4	9
33	Multi-body effects in a coarse-grained protein force field. *Journal of Chemical Physics*, **2021**, 154, 164113	3.9	9
32	Geometrical characterization of T cell receptor binding modes reveals class-specific binding to maximize access to antigen. *Proteins: Structure, Function and Bioinformatics*, **2020**, 88, 503-513	4.2	9
31	Grand canonical diffusion-influenced reactions: A stochastic theory with applications to multiscale reaction-diffusion simulations. *Journal of Chemical Physics*, **2018**, 149, 044102	3.9	8
30	Deflation reveals dynamical structure in nondominant reaction coordinates. *Journal of Chemical Physics*, **2019**, 151, 054103	3.9	8
29	Kernel methods for detecting coherent structures in dynamical data. *Chaos*, **2019**, 29, 123112	3.3	8
28	Discovery of a hidden transient state in all bromodomain families. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	8
27	Nanoscale coupling of endocytic pit growth and stability. *Science Advances*, **2019**, 5, eaax5775	14.3	7

26	Roadmap on Machine Learning in Electronic Structure. *Electronic Structure*,	2.6	7
25	Machine learning implicit solvation for molecular dynamics. *Journal of Chemical Physics*, **2021**, 155, 084101	3.9	6
24	Cyclization and Relaxation Dynamics of Finite-Length Collapsed Self-Avoiding Polymers. *Physical Review Letters*, **2019**, 122, 067801	7.4	5
23	Coupling of Conformational Switches in Calcium Sensor Unraveled with Local Markov Models and Transfer Entropy. *Journal of Chemical Theory and Computation*, **2020**, 16, 2584-2593	6.4	5
22	Polymer-like Model to Study the Dynamics of Dynamin Filaments on Deformable Membrane Tubes. *Biophysical Journal*, **2019**, 117, 1870-1891	2.9	5
21	Symmetric and antisymmetric kernels for machine learning problems in quantum physics and chemistry. *Machine Learning: Science and Technology*, **2021**, 2, 045016	5.1	5
20	Multiscale molecular kinetics by coupling Markov state models and reaction-diffusion dynamics. *Journal of Chemical Physics*, **2021**, 155, 124109	3.9	5
19	A scalable approach to the computation of invariant measures for high-dimensional Markovian systems. *Scientific Reports*, **2018**, 8, 1796	4.9	4
18	gr□ifai: interactive multiparameter optimization of molecules in a continuous vector space. *Bioinformatics*, **2020**, 36, 4093-4094	7.2	3
17	Response to comment "Transient complexes between dark rhodopsin and transducin: circumstantial evidence or physiological necessity?" by D. Dell'Orco and K.-W. Koch. *Biophysical Journal*, **2015**, 108, 778-9	2.9	3
16	Deeptime: a Python library for machine learning dynamical models from time series data. *Machine Learning: Science and Technology*,	5.1	3
15	Progress in deep Markov state modeling: Coarse graining and experimental data restraints. *Journal of Chemical Physics*, **2021**, 155, 214106	3.9	3
14	Convergence to the fixed-node limit in deep variational Monte Carlo. *Journal of Chemical Physics*, **2021**, 154, 124108	3.9	3
13	Independent Markov decomposition: Toward modeling kinetics of biomolecular complexes. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
12	Identifying optimal cycles in quantum thermal machines with reinforcement-learning. *Npj Quantum Information*, **2022**, 8,	8.6	2
11	Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. *Lecture Notes in Computer Science*, **2019**, 397-417	0.9	2
10	What Markov state models can and cannot do: Correlation versus path-based observables in protein folding models		2
9	Independent Markov Decomposition: Towards modeling kinetics of biomolecular complexes		2

8	Synergistic inhibition of SARS-CoV-2 cell entry by otamixaban and covalent protease inhibitors: pre-clinical assessment of pharmacological and molecular properties. *Chemical Science*, **2021**, 12, 12600-12609	9.4	2
7	Neural mode jump Monte Carlo. *Journal of Chemical Physics*, **2021**, 154, 074101	3.9	2
6	Coupling Particle-Based Reaction-Diffusion Simulations with Reservoirs Mediated by Reaction-Diffusion PDEs. *Multiscale Modeling and Simulation*, **2021**, 19, 1659-1683	1.8	1
5	Discovery of a hidden transient state in all bromodomain families		1
4	Hydrodynamic coupling for particle-based solvent-free membrane models. *Journal of Chemical Physics*, **2021**, 155, 114108	3.9	1
3	Parameterized Hypercomplex Graph Neural Networks for Graph Classification. *Lecture Notes in Computer Science*, **2021**, 204-216	0.9	1
2	Thermodynamics and Kinetics of Aggregation of Flexible Peripheral Membrane Proteins. *Journal of Physical Chemistry Letters*, **2021**, 12, 10497-10504	6.4	0
1	Computational tools for analysing structural changes in proteins in solution. *Applied Bioinformatics*, **2003**, 2, S11-7		