Fabian Paul

List of Publications by Year in Descending Order

18 papers	1,653 citations	13 h-index	21 g-index
21 ext. papers	2,217 ext. citations	6.9 avg, IF	4.87 L-index

#	Paper	IF	Citations
18	A critical perspective on Markov state model treatments of protein-protein association using coarse-grained simulations. *Journal of Chemical Physics*, **2021**, 154, 084101	3.9	2
17	Diversity of Long-Lived Intermediates along the Binding Pathway of Imatinib to Abl Kinase Revealed by MD Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 7852-7865	6.4	6
16	Polymerization and editing modes of a high-fidelity DNA polymerase are linked by a well-defined path. *Nature Communications*, **2020**, 11, 5379	17.4	9
15	Identification of Druggable Kinase Target Conformations Using Markov Model Metastable States Analysis of apo-Abl. *Journal of Chemical Theory and Computation*, **2020**, 16, 1896-1912	6.4	11
14	Variational selection of features for molecular kinetics. *Journal of Chemical Physics*, **2019**, 150, 194108	3.9	25
13	Identification of kinetic order parameters for non-equilibrium dynamics. *Journal of Chemical Physics* , **2019**, 150, 164120	3.9	15
12	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
11	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
10	Variational Koopman models: Slow collective variables and molecular kinetics from short off-equilibrium simulations. *Journal of Chemical Physics*, **2017**, 146, 154104	3.9	58
9	Predicting the Kinetics of RNA Oligonucleotides Using Markov State Models. *Journal of Chemical Theory and Computation*, **2017**, 13, 926-934	6.4	21
8	Protein-peptide association kinetics beyond the seconds timescale from atomistic simulations. *Nature Communications*, **2017**, 8, 1095	17.4	76
7	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
6	How to Distinguish Conformational Selection and Induced Fit Based on Chemical Relaxation Rates. *PLoS Computational Biology*, **2016**, 12, e1005067	5	43
5	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
4	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
3	Estimation and uncertainty of reversible Markov models. *Journal of Chemical Physics*, **2015**, 143, 174101	3.9	67
2	Conformational selection in protein binding and function. *Protein Science*, **2014**, 23, 1508-18	6.3	70

1	Identification of slow molecular order parameters for Markov model construction. *Journal of Chemical Physics*, **2013**, 139, 015102	3.9	522