Peter Kasson

List of Publications by Year in Descending Order

71 papers	6,500 citations	24 h-index	80 g-index
89 ext. papers	7,656 ext. citations	6.7 avg, IF	5.87 L-index

#	Paper	IF	Citations
71	gmxapi: A GROMACS-native Python interface for molecular dynamics with ensemble and plugin support.. *PLoS Computational Biology*, **2022**, 18, e1009835	5	
70	Development of COVID-19 vaccine using a dual Toll-like receptor ligand liposome adjuvant. *Npj Vaccines*, **2021**, 6, 137	9.5	2
69	The N-terminal Helix-Turn-Helix Motif of Transcription Factors MarA and Rob Drives DNA Recognition. *Journal of Physical Chemistry B*, **2021**, 125, 6791-6806	3.4	1
68	Inference of Joint Conformational Distributions from Separately Acquired Experimental Measurements. *Journal of Physical Chemistry Letters*, **2021**, 12, 1606-1611	6.4	2
67	Understanding Activation and Inhibition of SARS-CoV-2 Viral Entry with Single-Virus Microscopy. *Biophysical Journal*, **2021**, 120, 321a	2.9	78
66	Modeling biomolecular kinetics with large-scale simulation. *Current Opinion in Structural Biology*, **2021**, 72, 95-102	8.1	
65	Influenza hemagglutinin drives viral entry via two sequential intramembrane mechanisms. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 7200-7207	11.5	17
64	Managing Coronavirus Disease 2019 Spread With Voluntary Public Health Measures: Sweden as a Case Study for Pandemic Control. *Clinical Infectious Diseases*, **2020**, 71, 3174-3181	11.6	43
63	Acquired Functional Capsid Structures in Metazoan Totivirus-like dsRNA Virus. *Structure*, **2020**, 28, 888-896.e3	5.7	4
62	Adaptive Ensemble Biomolecular Applications at Scale. *SN Computer Science*, **2020**, 1, 1	2	2
61	SARS-CoV-2 receptor networks in diabetic and COVID-19-associated kidney disease. *Kidney International*, **2020**, 98, 1502-1518	9.9	33
60	Bilayer-Coated Nanoparticles Reveal How Influenza Viral Entry Depends on Membrane Deformability but Not Curvature. *Journal of Physical Chemistry Letters*, **2020**, 11, 7190-7196	6.4	3
59	Infectious Disease Research in the Era of Big Data. *Annual Review of Biomedical Data Science*, **2020**, 3, 43-59	5.6	4
58	Hybrid Refinement of Heterogeneous Conformational Ensembles Using Spectroscopic Data. *Journal of Physical Chemistry Letters*, **2019**, 10, 3410-3414	6.4	5
57	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. *Journal of Physical Chemistry B*, **2019**, 123, 3576-3590	3.4	7
56	Detecting and Controlling Dye Effects in Single-Virus Fusion Experiments. *Biophysical Journal*, **2019**, 117, 445-452	2.9	12
55	Antibiotic Uptake Across Gram-Negative Outer Membranes: Better Predictions Towards Better Antibiotics. *ACS Infectious Diseases*, **2019**, 5, 2096-2104	5.5	15

54	Conformational Intermediate That Controls KPC-2 Catalysis and Beta-Lactam Drug Resistance. *ACS Catalysis*, **2018**, 8, 2741-2747	13.1	13
53	Influenza Hemifusion Phenotype Depends on Membrane Context: Differences in Cell-Cell and Virus-Cell Fusion. *Journal of Molecular Biology*, **2018**, 430, 594-601	6.5	9
52	Cholesterol enhances influenza binding avidity by controlling nanoscale receptor clustering. *Chemical Science*, **2018**, 9, 2340-2347	9.4	29
51	Structural conservation in a membrane-enveloped filamentous virus infecting a hyperthermophilic acidophile. *Nature Communications*, **2018**, 9, 3360	17.4	18
50	Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. *Angewandte Chemie*, **2018**, 130, 17356-17360	3.6	0
49	Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. *Angewandte Chemie - International Edition*, **2018**, 57, 17110-17114	16.4	3
48	Predicting allostery and microbial drug resistance with molecular simulations. *Current Opinion in Structural Biology*, **2018**, 52, 80-86	8.1	6
47	Adaptive ensemble simulations of biomolecules. *Current Opinion in Structural Biology*, **2018**, 52, 87-94	8.1	14
46	pH Dependence of Zika Membrane Fusion Kinetics Reveals an Off-Pathway State. *ACS Central Science*, **2018**, 4, 1503-1510	16.8	19
45	gmxapi: a high-level interface for advanced control and extension of molecular dynamics simulations. *Bioinformatics*, **2018**, 34, 3945-3947	7.2	6
44	Predicting allosteric mutants that increase activity of a major antibiotic resistance enzyme. *Chemical Science*, **2017**, 8, 6484-6492	9.4	21
43	Model for a novel membrane envelope in a filamentous hyperthermophilic virus. *ELife*, **2017**, 6,	8.9	32
42	Disentangling Viral Membrane Fusion from Receptor Binding Using Synthetic DNA-Lipid Conjugates. *Biophysical Journal*, **2016**, 111, 123-31	2.9	23
41	Influenza viral membrane fusion is sensitive to sterol concentration but surprisingly robust to sterol chemical identity. *Scientific Reports*, **2016**, 6, 29842	4.9	19
40	Viral factors in influenza pandemic risk assessment. *ELife*, **2016**, 5,	8.9	61
39	Excess positional mutual information predicts both local and allosteric mutations affecting beta lactamase drug resistance. *Bioinformatics*, **2016**, 32, 3420-3427	7.2	11
38	Molecular simulation workflows as parallel algorithms: the execution engine of Copernicus, a distributed high-performance computing platform. *Journal of Chemical Theory and Computation*, **2015**, 11, 2600-8	6.4	31
37	Hemagglutinin Spatial Distribution Shifts in Response to Cholesterol in the Influenza Viral Envelope. *Biophysical Journal*, **2015**, 109, 1917-24	2.9	18

36	Coupled diffusion in lipid bilayers upon close approach. *Journal of the American Chemical Society*, **2015**, 137, 708-14	16.4	12
35	Dynamic heterogeneity controls diffusion and viscosity near biological interfaces. *Nature Communications*, **2014**, 5, 3034	17.4	48
34	Structure of the Neisserial outer membrane protein Opa□loop flexibility essential to receptor recognition and bacterial engulfment. *Journal of the American Chemical Society*, **2014**, 136, 9938-46	16.4	37
33	Ebolavirus entry requires a compact hydrophobic fist at the tip of the fusion loop. *Journal of Virology*, **2014**, 88, 6636-49	6.6	33
32	Improving pandemic influenza risk assessment. *ELife*, **2014**, 3, e03883	8.9	45
31	Lipid converter, a framework for lipid manipulations in molecular dynamics simulations. *Journal of Membrane Biology*, **2014**, 247, 1137-40	2.3	5
30	Author response: Improving pandemic influenza risk assessment **2014**,		2
29	Probing microscopic material properties inside simulated membranes through spatially resolved three-dimensional local pressure fields and surface tensions. *Chemistry and Physics of Lipids*, **2013**, 169, 106-12	3.7	10
28	Multiphasic effects of cholesterol on influenza fusion kinetics reflect multiple mechanistic roles. *Biophysical Journal*, **2013**, 105, 1383-7	2.9	30
27	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. *Bioinformatics*, **2013**, 29, 845-54	7.2	4786
26	Lipid tail protrusion in simulations predicts fusogenic activity of influenza fusion peptide mutants and conformational models. *PLoS Computational Biology*, **2013**, 9, e1002950	5	64
25	Receptor binding by influenza virus: using computational techniques to extend structural data. *Biochemistry*, **2012**, 51, 2359-65	3.2	6
24	Water ordering at membrane interfaces controls fusion dynamics. *Journal of the American Chemical Society*, **2011**, 133, 3812-5	16.4	41
23	A bundling of viral fusion mechanisms. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 3827-8	11.5	4
22	Copernicus **2011**,		19
21	Atomic-resolution simulations predict a transition state for vesicle fusion defined by contact of a few lipid tails. *PLoS Computational Biology*, **2010**, 6, e1000829	5	94
20	"Cross-graining": efficient multi-scale simulation via Markov state models. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2010**, 260-8	1.3	1
19	Combining molecular dynamics with bayesian analysis to predict and evaluate ligand-binding mutations in influenza hemagglutinin. *Journal of the American Chemical Society*, **2009**, 131, 11338-40	16.4	26

18	Combining mutual information with structural analysis to screen for functionally important residues in influenza hemagglutinin. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2009**, 492-503	1.3	4
17	Structural basis for influence of viral glycans on ligand binding by influenza hemagglutinin. *Biophysical Journal*, **2008**, 95, L48-50	2.9	20
16	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. *PLoS Computational Biology*, **2007**, 3, e220	5	91
15	Persistent voids: a new structural metric for membrane fusion. *Bioinformatics*, **2007**, 23, 1753-9	7.2	44
14	Heterogeneity even at the speed limit of folding: large-scale molecular dynamics study of a fast-folding variant of the villin headpiece. *Journal of Molecular Biology*, **2007**, 374, 806-16	6.5	154
13	Predicting structure and dynamics of loosely-ordered protein complexes: influenza hemagglutinin fusion peptide. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2007**, 40-50	1.3	4
12	Ensemble molecular dynamics yields submillisecond kinetics and intermediates of membrane fusion. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 11916-21	11.5	124
11	A hybrid machine-learning approach for segmentation of protein localization data. *Bioinformatics*, **2005**, 21, 3778-86	7.2	10
10	Quantitative imaging of lymphocyte membrane protein reorganization and signaling. *Biophysical Journal*, **2005**, 88, 579-89	2.9	6
9	Deformable modeling for improved calculation of molecular velocities from single-particle tracking **2005**, 208-11		
8	Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. *PLoS Computational Biology*, **2005**, preprint, e220	5	1
7	Molecular dynamics simulation of lipid reorientation at bilayer edges. *Biophysical Journal*, **2004**, 86, 3744-9	2.9	24
6	Kinetics of peptide binding to the class II MHC protein I-Ek. *Biochemistry*, **2000**, 39, 1048-58	3.2	47
5	Formation of a highly peptide-receptive state of class II MHC. *Immunity*, **1998**, 9, 699-709	32.3	122
4	Influenza hemagglutinin drives viral entry via two sequential intramembrane mechanisms		2
3	Intervention strategies against COVID-19 and their estimated impact on Swedish healthcare capacity		15
2	Precise triggering and chemical control of single-virus fusion within endosomes		1
1	Single-virus fusion measurements yield an opportunistic model for SARS-CoV-2 fusion		1