# Peter Kasson

## List of Publications by Citations



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|---|---|---|---|
| 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 | GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. *Bioinformatics*, **2013**, 29, 845-54 | 7.2 | 4786 |
| 70 | 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 |
| 69 | 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 |
| 68 | Formation of a highly peptide-receptive state of class II MHC. *Immunity*, **1998**, 9, 699-709 | 32.3 | 122 |
| 67 | 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 |
| 66 | Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. *PLoS Computational Biology*, **2007**, 3, e220 | 5 | 91 |
| 65 | Understanding Activation and Inhibition of SARS-CoV-2 Viral Entry with Single-Virus Microscopy. *Biophysical Journal*, **2021**, 120, 321a | 2.9 | 78 |
| 64 | Lipid tail protrusion in simulations predicts fusogenic activity of influenza fusion peptide mutants and conformational models. *PLoS Computational Biology*, **2013**, 9, e1002950 | 5 | 64 |
| 63 | Viral factors in influenza pandemic risk assessment. *ELife*, **2016**, 5, | 8.9 | 61 |
| 62 | Dynamic heterogeneity controls diffusion and viscosity near biological interfaces. *Nature Communications*, **2014**, 5, 3034 | 17.4 | 48 |
| 61 | Kinetics of peptide binding to the class II MHC protein I-Ek. *Biochemistry*, **2000**, 39, 1048-58 | 3.2 | 47 |
| 60 | Improving pandemic influenza risk assessment. *ELife*, **2014**, 3, e03883 | 8.9 | 45 |
| 59 | Persistent voids: a new structural metric for membrane fusion. *Bioinformatics*, **2007**, 23, 1753-9 | 7.2 | 44 |
| 58 | 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 |
| 57 | Water ordering at membrane interfaces controls fusion dynamics. *Journal of the American Chemical Society*, **2011**, 133, 3812-5 | 16.4 | 41 |
| 56 | 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 |
| 55 | Ebolavirus entry requires a compact hydrophobic fist at the tip of the fusion loop. *Journal of Virology*, **2014**, 88, 6636-49 | 6.6 | 33 |

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| 54 | SARS-CoV-2 receptor networks in diabetic and COVID-19-associated kidney disease. *Kidney International*, **2020**, 98, 1502-1518 | 9.9 | 33 |
| 53 | Model for a novel membrane envelope in a filamentous hyperthermophilic virus. *ELife*, **2017**, 6, | 8.9 | 32 |
| 52 | 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 |
| 51 | Multiphasic effects of cholesterol on influenza fusion kinetics reflect multiple mechanistic roles. *Biophysical Journal*, **2013**, 105, 1383-7 | 2.9 | 30 |
| 50 | Cholesterol enhances influenza binding avidity by controlling nanoscale receptor clustering. *Chemical Science*, **2018**, 9, 2340-2347 | 9.4 | 29 |
| 49 | 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 |
| 48 | Molecular dynamics simulation of lipid reorientation at bilayer edges. *Biophysical Journal*, **2004**, 86, 3744-9 | 2.9 | 24 |
| 47 | Disentangling Viral Membrane Fusion from Receptor Binding Using Synthetic DNA-Lipid Conjugates. *Biophysical Journal*, **2016**, 111, 123-31 | 2.9 | 23 |
| 46 | Predicting allosteric mutants that increase activity of a major antibiotic resistance enzyme. *Chemical Science*, **2017**, 8, 6484-6492 | 9.4 | 21 |
| 45 | Structural basis for influence of viral glycans on ligand binding by influenza hemagglutinin. *Biophysical Journal*, **2008**, 95, L48-50 | 2.9 | 20 |
| 44 | Influenza viral membrane fusion is sensitive to sterol concentration but surprisingly robust to sterol chemical identity. *Scientific Reports*, **2016**, 6, 29842 | 4.9 | 19 |
| 43 | Copernicus **2011**, | | 19 |
| 42 | pH Dependence of Zika Membrane Fusion Kinetics Reveals an Off-Pathway State. *ACS Central Science*, **2018**, 4, 1503-1510 | 16.8 | 19 |
| 41 | Hemagglutinin Spatial Distribution Shifts in Response to Cholesterol in the Influenza Viral Envelope. *Biophysical Journal*, **2015**, 109, 1917-24 | 2.9 | 18 |
| 40 | Structural conservation in a membrane-enveloped filamentous virus infecting a hyperthermophilic acidophile. *Nature Communications*, **2018**, 9, 3360 | 17.4 | 18 |
| 39 | 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 |
| 38 | Antibiotic Uptake Across Gram-Negative Outer Membranes: Better Predictions Towards Better Antibiotics. *ACS Infectious Diseases*, **2019**, 5, 2096-2104 | 5.5 | 15 |
| 37 | Intervention strategies against COVID-19 and their estimated impact on Swedish healthcare capacity | | 15 |

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| 36 | Adaptive ensemble simulations of biomolecules. *Current Opinion in Structural Biology*, **2018**, 52, 87-94 | 8.1 | 14 |
| 35 | Conformational Intermediate That Controls KPC-2 Catalysis and Beta-Lactam Drug Resistance. *ACS Catalysis*, **2018**, 8, 2741-2747 | 13.1 | 13 |
| 34 | Detecting and Controlling Dye Effects in Single-Virus Fusion Experiments. *Biophysical Journal*, **2019**, 117, 445-452 | 2.9 | 12 |
| 33 | Coupled diffusion in lipid bilayers upon close approach. *Journal of the American Chemical Society*, **2015**, 137, 708-14 | 16.4 | 12 |
| 32 | Excess positional mutual information predicts both local and allosteric mutations affecting beta lactamase drug resistance. *Bioinformatics*, **2016**, 32, 3420-3427 | 7.2 | 11 |
| 31 | 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 |
| 30 | A hybrid machine-learning approach for segmentation of protein localization data. *Bioinformatics*, **2005**, 21, 3778-86 | 7.2 | 10 |
| 29 | 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 |
| 28 | 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 |
| 27 | Receptor binding by influenza virus: using computational techniques to extend structural data. *Biochemistry*, **2012**, 51, 2359-65 | 3.2 | 6 |
| 26 | Quantitative imaging of lymphocyte membrane protein reorganization and signaling. *Biophysical Journal*, **2005**, 88, 579-89 | 2.9 | 6 |
| 25 | Predicting allostery and microbial drug resistance with molecular simulations. *Current Opinion in Structural Biology*, **2018**, 52, 80-86 | 8.1 | 6 |
| 24 | gmxapi: a high-level interface for advanced control and extension of molecular dynamics simulations. *Bioinformatics*, **2018**, 34, 3945-3947 | 7.2 | 6 |
| 23 | Hybrid Refinement of Heterogeneous Conformational Ensembles Using Spectroscopic Data. *Journal of Physical Chemistry Letters*, **2019**, 10, 3410-3414 | 6.4 | 5 |
| 22 | Lipid converter, a framework for lipid manipulations in molecular dynamics simulations. *Journal of Membrane Biology*, **2014**, 247, 1137-40 | 2.3 | 5 |
| 21 | Acquired Functional Capsid Structures in Metazoan Totivirus-like dsRNA Virus. *Structure*, **2020**, 28, 888-896.e3 | 5.2 | 4 |
| 20 | 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 |
| 19 | 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 |

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| 18 | Infectious Disease Research in the Era of Big Data. *Annual Review of Biomedical Data Science*, **2020**, 3, 43-59 | 5.6 | 4 |
| 17 | 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 |
| 16 | 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 |
| 15 | Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. *Angewandte Chemie - International Edition*, **2018**, 57, 17110-17114 | 16.4 | 3 |
| 14 | Adaptive Ensemble Biomolecular Applications at Scale. *SN Computer Science*, **2020**, 1, 1 | 2 | 2 |
| 13 | Development of COVID-19 vaccine using a dual Toll-like receptor ligand liposome adjuvant. *Npj Vaccines*, **2021**, 6, 137 | 9.5 | 2 |
| 12 | Influenza hemagglutinin drives viral entry via two sequential intramembrane mechanisms | | 2 |
| 11 | Author response: Improving pandemic influenza risk assessment **2014**, | | 2 |
| 10 | Inference of Joint Conformational Distributions from Separately Acquired Experimental Measurements. *Journal of Physical Chemistry Letters*, **2021**, 12, 1606-1611 | 6.4 | 2 |
| 9 | Control of membrane fusion mechanism by lipid composition: predictions from ensemble molecular dynamics. *PLoS Computational Biology*, **2005**, preprint, e220 | 5 | 1 |
| 8 | Precise triggering and chemical control of single-virus fusion within endosomes | | 1 |
| 7 | Single-virus fusion measurements yield an opportunistic model for SARS-CoV-2 fusion | | 1 |
| 6 | 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 |
| 5 | "Cross-graining": efficient multi-scale simulation via Markov state models. *Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing*, **2010**, 260-8 | 1.3 | 1 |
| 4 | Refinement of Highly Flexible Protein Structures using Simulation-Guided Spectroscopy. *Angewandte Chemie*, **2018**, 130, 17356-17360 | 3.6 | 0 |
| 3 | Deformable modeling for improved calculation of molecular velocities from single-particle tracking **2005**, 208-11 | | |
| 2 | Modeling biomolecular kinetics with large-scale simulation. *Current Opinion in Structural Biology*, **2021**, 72, 95-102 | 8.1 | |
| 1 | gmxapi: A GROMACS-native Python interface for molecular dynamics with ensemble and plugin support.. *PLoS Computational Biology*, **2022**, 18, e1009835 | 5 | |