Jochen Hub

List of Publications by Citations

72 papers	5,610 citations	29 h-index	74 g-index
86 ext. papers	6,636 ext. citations	7.4 avg, IF	6.06 L-index

#	Paper	IF	Citations
72	Molecular anatomy of a trafficking organelle. *Cell*, **2006**, 127, 831-46	56.2	1670
71	g_wham—A Free Weighted Histogram Analysis Implementation Including Robust Error and Autocorrelation Estimates. *Journal of Chemical Theory and Computation*, **2010**, 6, 3713-3720	6.4	930
70	Force Field Benchmark of Organic Liquids: Density, Enthalpy of Vaporization, Heat Capacities, Surface Tension, Isothermal Compressibility, Volumetric Expansion Coefficient, and Dielectric Constant. *Journal of Chemical Theory and Computation*, **2012**, 8, 61-74	6.4	476
69	Mechanism of selectivity in aquaporins and aquaglyceroporins. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 1198-203	11.5	328
68	Atomistic simulation of ion solvation in water explains surface preference of halides. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 6838-6842	11.5	171
67	Large influence of cholesterol on solute partitioning into lipid membranes. *Journal of the American Chemical Society*, **2012**, 134, 5351-61	16.4	124
66	Quantifying Artifacts in Ewald Simulations of Inhomogeneous Systems with a Net Charge. *Journal of Chemical Theory and Computation*, **2014**, 10, 381-90	6.4	121
65	Does CO2 permeate through aquaporin-1?. *Biophysical Journal*, **2006**, 91, 842-8	2.9	118
64	Detection of functional modes in protein dynamics. *PLoS Computational Biology*, **2009**, 5, e1000480	5	107
63	WAXSiS: a web server for the calculation of SAXS/WAXS curves based on explicit-solvent molecular dynamics. *Nucleic Acids Research*, **2015**, 43, W225-30	20.1	96
62	Validating solution ensembles from molecular dynamics simulation by wide-angle X-ray scattering data. *Biophysical Journal*, **2014**, 107, 435-447	2.9	82
61	Potentials of mean force and permeabilities for carbon dioxide, ammonia, and water flux across a Rhesus protein channel and lipid membranes. *Journal of the American Chemical Society*, **2010**, 132, 13251-63	16.4	78
60	Dynamics and energetics of permeation through aquaporins. What do we learn from molecular dynamics simulations?. *Handbook of Experimental Pharmacology*, **2009**, 57-76	3.2	76
59	Interpretation of solution x-ray scattering by explicit-solvent molecular dynamics. *Biophysical Journal*, **2015**, 108, 2573-2584	2.9	72
58	Short-range order and collective dynamics of DMPC bilayers: a comparison between molecular dynamics simulations, X-ray, and neutron scattering experiments. *Biophysical Journal*, **2007**, 93, 3156-68	2.9	72
57	Interpreting solution X-ray scattering data using molecular simulations. *Current Opinion in Structural Biology*, **2018**, 49, 18-26	8.1	63
56	Time-resolved WAXS reveals accelerated conformational changes in iodoretinal-substituted proteorhodopsin. *Biophysical Journal*, **2011**, 101, 1345-53	2.9	54

55	Local partition coefficients govern solute permeability of cholesterol-containing membranes. *Biophysical Journal*, **2013**, 105, 2760-70	2.9	53
54	Voltage-regulated water flux through aquaporin channels in silico. *Biophysical Journal*, **2010**, 99, L97-9	2.9	49
53	Partial least-squares functional mode analysis: application to the membrane proteins AQP1, Aqy1, and CLC-ec1. *Biophysical Journal*, **2012**, 103, 786-96	2.9	48
52	Spontaneous quaternary and tertiary T-R transitions of human hemoglobin in molecular dynamics simulation. *PLoS Computational Biology*, **2010**, 6, e1000774	5	48
51	MemGen: a general web server for the setup of lipid membrane simulation systems. *Bioinformatics*, **2015**, 31, 2897-9	7.2	44
50	Organic molecules on the surface of water droplets--an energetic perspective. *Physical Chemistry Chemical Physics*, **2012**, 14, 9537-45	3.6	43
49	Thermodynamics of hydronium and hydroxide surface solvation. *Chemical Science*, **2014**, 5, 1745	9.4	42
48	Simulations of Pore Formation in Lipid Membranes: Reaction Coordinates, Convergence, Hysteresis, and Finite-Size Effects. *Journal of Chemical Theory and Computation*, **2016**, 12, 3261-9	6.4	40
47	CO2 and O2 distribution in Rubisco suggests the small subunit functions as a CO2 reservoir. *Journal of the American Chemical Society*, **2014**, 136, 3165-71	16.4	39
46	A glycerophospholipid-specific pocket in the RVFV class II fusion protein drives target membrane insertion. *Science*, **2017**, 358, 663-667	33.3	35
45	Ultrafast anisotropic protein quake propagation after CO photodissociation in myoglobin. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 10565-70	11.5	35
44	Bayesian refinement of protein structures and ensembles against SAXS data using molecular dynamics. *PLoS Computational Biology*, **2017**, 13, e1005800	5	34
43	Is TEA an inhibitor for human Aquaporin-1?. *Pflugers Archiv European Journal of Physiology*, **2008**, 456, 663-9	4.6	29
42	Disentangling polydispersity in the PCNA-p15PAF complex, a disordered, transient and multivalent macromolecular assembly. *Nucleic Acids Research*, **2017**, 45, 1501-1515	20.1	28
41	SAXS-Restrained Ensemble Simulations of Intrinsically Disordered Proteins with Commitment to the Principle of Maximum Entropy. *Journal of Chemical Theory and Computation*, **2019**, 15, 5103-5115	6.4	27
40	Accelerating potential of mean force calculations for lipid membrane permeation: System size, reaction coordinate, solute-solute distance, and cutoffs. *Journal of Chemical Physics*, **2016**, 145, 125101	3.9	24
39	Metastable Prepores in Tension-Free Lipid Bilayers. *Physical Review Letters*, **2018**, 120, 128103	7.4	23
38	Combined Small-Angle X-ray and Neutron Scattering Restraints in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 4687-4698	6.4	23

37	Structural Properties of Protein-Detergent Complexes from SAXS and MD Simulations. *Journal of Physical Chemistry Letters*, **2015**, 6, 5116-21	6.4	23
36	Rationalizing Steroid Interactions with Lipid Membranes: Conformations, Partitioning, and Kinetics. *ACS Central Science*, **2018**, 4, 1155-1165	16.8	22
35	Dynamics and energetics of solute permeation through the Plasmodium falciparum aquaglyceroporin. *Physical Chemistry Chemical Physics*, **2010**, 12, 10246-54	3.6	22
34	Probing a Continuous Polar Defect: A Reaction Coordinate for Pore Formation in Lipid Membranes. *Journal of Chemical Theory and Computation*, **2017**, 13, 2352-2366	6.4	21
33	Molecular Mechanism of Polycation-Induced Pore Formation in Biomembranes. *ACS Biomaterials Science and Engineering*, **2019**, 5, 780-794	5.5	19
32	The Lipid Bilayer Provides a Site for Cortisone Crystallization at High Cortisone Concentrations. *Scientific Reports*, **2016**, 6, 22425	4.9	18
31	Energetics and mechanism of anion permeation across formate-nitrite transporters. *Scientific Reports*, **2017**, 7, 12027	4.9	16
30	Computer simulations of protein-membrane systems. *Progress in Molecular Biology and Translational Science*, **2020**, 170, 273-403	4	15
29	Quantifying Lateral Inhomogeneity of Cholesterol-Containing Membranes. *Journal of Physical Chemistry Letters*, **2015**, 6, 4799-803	6.4	13
28	Small-Angle X-ray Scattering Curves of Detergent Micelles: Effects of Asymmetry, Shape Fluctuations, Disorder, and Atomic Details. *Journal of Physical Chemistry Letters*, **2020**, 11, 945-951	6.4	12
27	g_permute: Permutation-reduced phase space density compaction. *Computer Physics Communications*, **2009**, 180, 455-458	4.2	11
26	Not only enthalpy: large entropy contribution to ion permeation barriers in single-file channels. *Biophysical Journal*, **2008**, 95, 2275-82	2.9	11
25	Observing the Structural Evolution in the Photodissociation of Diiodomethane with Femtosecond Solution X-Ray Scattering. *Physical Review Letters*, **2020**, 125, 226001	7.4	10
24	Merging In-Solution X-ray and Neutron Scattering Data Allows Fine Structural Analysis of Membrane-Protein Detergent Complexes. *Journal of Physical Chemistry Letters*, **2018**, 9, 3910-3914	6.4	10
23	Temperature-Dependent Atomic Models of Detergent Micelles Refined against Small-Angle X-Ray Scattering Data. *Angewandte Chemie - International Edition*, **2018**, 57, 5635-5639	16.4	9
22	Free energies of membrane stalk formation from a lipidomics perspective. *Nature Communications*, **2021**, 12, 6594	17.4	7
21	An allosteric interaction controls the activation mechanism of SHP2 tyrosine phosphatase. *Scientific Reports*, **2020**, 10, 18530	4.9	7
20	How arginine derivatives alter the stability of lipid membranes: dissecting the roles of side chains, backbone and termini. *European Biophysics Journal*, **2021**, 50, 127-142	1.9	7

19	Quantifying the influence of the ion cloud on SAXS profiles of charged proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 26351-26361	3.6	7
18	Potential of Mean Force Calculations of Solute Permeation Across UT-B and AQP1: A Comparison between Molecular Dynamics and 3D-RISM. *Journal of Physical Chemistry B*, **2017**, 121, 1506-1519	3.4	6
17	Structural Determinants of Phosphopeptide Binding to the N-Terminal Src Homology 2 Domain of the SHP2 Phosphatase. *Journal of Chemical Information and Modeling*, **2020**, 60, 3157-3171	6.1	6
16	Comment on "Molecular selectivity in aquaporin channels studied by the 3D-RISM theory". *Journal of Physical Chemistry B*, **2011**, 115, 8364-6; discussion 8367-9	3.4	5
15	Three- and four-site models for heavy water: SPC/E-HW, TIP3P-HW, and TIP4P/2005-HW. *Journal of Chemical Physics*, **2021**, 154, 194501	3.9	4
14	Anisotropic time-resolved solution X-ray scattering patterns from explicit-solvent molecular dynamics. *Journal of Chemical Physics*, **2015**, 143, 104108	3.9	3
13	Lipid Droplets Embedded in a Model Cell Membrane Create a Phospholipid Diffusion Barrier.. *Small*, **2022**, e2106524	11	2
12	Cooperative Effects of an Antifungal Moiety and DMSO on Pore Formation over Lipid Membranes Revealed by Free Energy Calculations. *Journal of Physical Chemistry B*, **2020**, 124, 8811-8821	3.4	2
11	The structure of Prp2 bound to RNA and ADP-BeF reveals structural features important for RNA unwinding by DEAH-box ATPases. *Acta Crystallographica Section D: Structural Biology*, **2021**, 77, 496-509	5.5	2
10	The loops of the N-SH2 binding cleft do not serve as allosteric switch in SHP2 activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	2
9	Joint Reaction Coordinate for Computing the Free-Energy Landscape of Pore Nucleation and Pore Expansion in Lipid Membranes. *Journal of Chemical Theory and Computation*, **2021**, 17, 1229-1239	6.4	2
8	Steroid-steroid interactions in biological membranes: Cholesterol and cortisone. *Chemistry and Physics of Lipids*, **2019**, 221, 193-197	3.7	1
7	Free-Energy Calculations of Pore Formation in Lipid Membranes **2019**, 109-124		1
6	Assigning crystallographic electron densities with free energy calculations-The case of the fluoride channel Fluc. *PLoS ONE*, **2018**, 13, e0196751	3.7	0
5	Structure and dynamics of the quaternary hunchback mRNA translation repression complex. *Nucleic Acids Research*, **2021**, 49, 8866-8885	20.1	0
4	Temperature-Dependent Atomic Models of Detergent Micelles Refined against Small-Angle X-Ray Scattering Data. *Angewandte Chemie*, **2018**, 130, 5737-5741	3.6	
3	Unexpected Effects of Cholesterol on Membrane Permeability. *Biophysical Journal*, **2013**, 104, 192a-193a	2.9	
2	Interpreting SAXS/WAXS Data with Explicit-Solvent Simulations: A Practical Guide. *Methods in Molecular Biology*, **2020**, 2168, 199-215	1.4	

1 Propensity, free energy contributions and conformation of primary n-alcohols at a water surface. *Physical Chemistry Chemical Physics*, **2021**, 23, 18823-18829 3.6