Berk Hess

List of Publications by Citations

45 papers	38,714 citations	27 h-index	49 g-index
49 ext. papers	44,484 ext. citations	4.9 avg, IF	7.51 L-index

#	Paper	IF	Citations
45	GROMACS 4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. *Journal of Chemical Theory and Computation*, **2008**, 4, 435-47	6.4	11706
44	GROMACS: fast, flexible, and free. *Journal of Computational Chemistry*, **2005**, 26, 1701-18	3.5	10273
43	LINCS: A linear constraint solver for molecular simulations. *Journal of Computational Chemistry*, **1997**, 18, 1463-1472	3.5	10241
42	P-LINCS: A Parallel Linear Constraint Solver for Molecular Simulation. *Journal of Chemical Theory and Computation*, **2008**, 4, 116-22	6.4	2072
41	Improving efficiency of large time-scale molecular dynamics simulations of hydrogen-rich systems. *Journal of Computational Chemistry*, **1999**, 20, 786-798	3.5	618
40	Implementation of the CHARMM Force Field in GROMACS: Analysis of Protein Stability Effects from Correction Maps, Virtual Interaction Sites, and Water Models. *Journal of Chemical Theory and Computation*, **2010**, 6, 459-66	6.4	600
39	Determining the shear viscosity of model liquids from molecular dynamics simulations. *Journal of Chemical Physics*, **2002**, 116, 209	3.9	509
38	A flexible algorithm for calculating pair interactions on SIMD architectures. *Computer Physics Communications*, **2013**, 184, 2641-2650	4.2	347
37	Hydration thermodynamic properties of amino acid analogues: a systematic comparison of biomolecular force fields and water models. *Journal of Physical Chemistry B*, **2006**, 110, 17616-26	3.4	271
36	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. *Journal of the American Chemical Society*, **2004**, 126, 4228-33	16.4	246
35	Similarities between principal components of protein dynamics and random diffusion. *Physical Review E*, **2000**, 62, 8438-48	2.4	234
34	Cation specific binding with protein surface charges. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 13296-300	11.5	209
33	Reproducible polypeptide folding and structure prediction using molecular dynamics simulations. *Journal of Molecular Biology*, **2005**, 354, 173-83	6.5	150
32	Osmotic coefficients of atomistic NaCl (aq) force fields. *Journal of Chemical Physics*, **2006**, 124, 164509	3.9	122
31	Analysis and evaluation of channel models: simulations of alamethicin. *Biophysical Journal*, **2002**, 83, 2393-407	2.9	117
30	Long time atomistic polymer trajectories from coarse grained simulations: bisphenol-A polycarbonate. *Soft Matter*, **2006**, 2, 409-414	3.6	115
29	Modeling multibody effects in ionic solutions with a concentration dependent dielectric permittivity. *Physical Review Letters*, **2006**, 96, 147801	7.4	104

28	Lennard-Jones Lattice Summation in Bilayer Simulations Has Critical Effects on Surface Tension and Lipid Properties. *Journal of Chemical Theory and Computation*, **2013**, 9, 3527-37	6.4	89
27	Direct-Space Corrections Enable Fast and Accurate Lorentz-Berthelot Combination Rule Lennard-Jones Lattice Summation. *Journal of Chemical Theory and Computation*, **2015**, 11, 5737-46	6.4	70
26	Competing adsorption between hydrated peptides and water onto metal surfaces: from electronic to conformational properties. *Journal of the American Chemical Society*, **2008**, 130, 13460-4	16.4	67
25	Dynamics and structure of Ln(III)-aqua ions: a comparative molecular dynamics study using ab initio based flexible and polarizable model potentials. *Journal of Physical Chemistry B*, **2009**, 113, 7270-81	3.4	59
24	An application of flexible constraints in Monte Carlo simulations of the isobaric--isothermal ensemble of liquid water and ice Ih with the polarizable and flexible mobile charge densities in harmonic oscillators model. *Journal of Chemical Physics*, **2004**, 120, 11133-43	3.9	49
23	Heterogeneous parallelization and acceleration of molecular dynamics simulations in GROMACS. *Journal of Chemical Physics*, **2020**, 153, 134110	3.9	46
22	Ion pairing in aqueous electrolyte solutions with biologically relevant anions. *Journal of Physical Chemistry B*, **2011**, 115, 3734-9	3.4	43
21	3□helix conformation facilitates the transition of a voltage sensor S4 segment toward the down state. *Biophysical Journal*, **2011**, 100, 1446-54	2.9	40
20	GROMACS□he road ahead. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 710-715	7.9	38
19	Fast-Growth Thermodynamic Integration: Calculating Excess Chemical Potentials of Additive Molecules in Polymer Microstructures. *Macromolecules*, **2008**, 41, 2283-2289	5.5	31
18	Flexible constraints: An adiabatic treatment of quantum degrees of freedom, with application to the flexible and polarizable mobile charge densities in harmonic oscillators model for water. *Journal of Chemical Physics*, **2002**, 116, 9602-9610	3.9	27
17	Algorithm improvements for molecular dynamics simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 93-108	7.9	26
16	Further investigation on the validity of Stokes□Einstein behaviour at the molecular level. *Chemical Physics Letters*, **2001**, 334, 337-342	2.5	22
15	Sequence dependency of canonical base pair opening in the DNA double helix. *PLoS Computational Biology*, **2017**, 13, e1005463	5	21
14	Modeling Solubilities of Additives in Polymer Microstructures: Single-Step Perturbation Method Based on a Soft-Cavity Reference State. *Macromolecules*, **2008**, 41, 5055-5061	5.5	20
13	Driving forces for adsorption of amphiphilic peptides to the air-water interface. *Journal of Physical Chemistry B*, **2010**, 114, 11093-101	3.4	19
12	Molecular origin of contact line friction in dynamic wetting. *Physical Review Fluids*, **2018**, 3,	2.8	19
11	Water□ubstrate physico-chemistry in wetting dynamics. *Journal of Fluid Mechanics*, **2015**, 781, 695-711	3.7	16

10	Predictive Modeling of Phenol Chemical Potentials in Molten Bisphenol A Polycarbonate over a Broad Temperature Range. *Macromolecules*, **2008**, 41, 7281-7283	5.5	15
9	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
8	Riemann metric approach to optimal sampling of multidimensional free-energy landscapes. *Physical Review E*, **2018**, 98, 023312	2.4	10
7	Stability of Hydrophobically Modified Poly(p-phenylenesulfonate) Bundles As Observed by Molecular Dynamics Simulation. *Macromolecules*, **2007**, 40, 1703-1707	5.5	9
6	Regularizing the fast multipole method for use in molecular simulation. *Journal of Chemical Physics*, **2019**, 151, 234113	3.9	5
5	Chain packing in polycarbonate glasses. *Journal of Chemical Physics*, **2010**, 132, 104901	3.9	4
4	The accelerated weight histogram method for alchemical free energy calculations. *Journal of Chemical Physics*, **2021**, 154, 204103	3.9	4
3	Interaction of water with N,N′1,2-ethanediyl-bis(6-hydroxy-hexanamide) crystals: a simulation study. *Journal of Physical Chemistry B*, **2009**, 113, 627-31	3.4	3
2	Predictions of Skin Permeability Using Molecular Dynamics Simulation from Two-Dimensional Sampling of Spatial and Alchemical Perturbation Reaction Coordinates		2
1	Electrowetting diminishes contact line friction in molecular wetting. *Physical Review Fluids*, **2020**, 5,	2.8	2