# Berk Hess

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5983798/publications.pdf

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| 46 | 49,762 | 172207 | 223531 |
|---|---|---|---|
| papers | citations | 29 h-index | 46 g-index |

| 49 | 49 | 49 | 38304 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | GROMACS 4:â€‰ Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 435-447. | 2.3 | 13,875 |
| 2 | GROMACS: Fast, flexible, and free. Journal of Computational Chemistry, 2005, 26, 1701-1718. | 1.5 | 13,676 |
| 3 | LINCS: A linear constraint solver for molecular simulations. Journal of Computational Chemistry, 1997, 18, 1463-1472. | 1.5 | 13,446 |
| 4 | P-LINCS:â€‰ A Parallel Linear Constraint Solver for Molecular Simulation. Journal of Chemical Theory and Computation, 2008, 4, 116-122. | 2.3 | 2,976 |
| 5 | 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, 459-466. | 2.3 | 866 |
| 6 | Improving efficiency of large time-scale molecular dynamics simulations of hydrogen-rich systems. Journal of Computational Chemistry, 1999, 20, 786-798. | 1.5 | 779 |
| 7 | Determining the shear viscosity of model liquids from molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 209. | 1.2 | 620 |
| 8 | A flexible algorithm for calculating pair interactions on SIMD architectures. Computer Physics Communications, 2013, 184, 2641-2650. | 3.0 | 544 |
| 9 | Hydration Thermodynamic Properties of Amino Acid Analogues:Â A Systematic Comparison of Biomolecular Force Fields and Water Models. Journal of Physical Chemistry B, 2006, 110, 17616-17626. | 1.2 | 305 |
| 10 | Similarities between principal components of protein dynamics and random diffusion. Physical Review E, 2000, 62, 8438-8448. | 0.8 | 276 |
| 11 | Heterogeneous parallelization and acceleration of molecular dynamics simulations in GROMACS. Journal of Chemical Physics, 2020, 153, 134110. | 1.2 | 275 |
| 12 | Photoactivation of the Photoactive Yellow Protein:Â Why Photon Absorption Triggers a Trans-to-Cis Isomerization of the Chromophore in the Protein. Journal of the American Chemical Society, 2004, 126, 4228-4233. | 6.6 | 265 |
| 13 | Cation specific binding with protein surface charges. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13296-13300. | 3.3 | 226 |
| 14 | Reproducible Polypeptide Folding and Structure Prediction using Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 354, 173-183. | 2.0 | 165 |
| 15 | Lennard-Jones Lattice Summation in Bilayer Simulations Has Critical Effects on Surface Tension and Lipid Properties. Journal of Chemical Theory and Computation, 2013, 9, 3527-3537. | 2.3 | 138 |
| 16 | Osmotic coefficients of atomistic NaCl (aq) force fields. Journal of Chemical Physics, 2006, 124, 164509. | 1.2 | 132 |
| 17 | Analysis and Evaluation of Channel Models: Simulations of Alamethicin. Biophysical Journal, 2002, 83, 2393-2407. | 0.2 | 123 |
| 18 | Long time atomistic polymer trajectories from coarse grained simulations: bisphenol-A polycarbonate. Soft Matter, 2006, 2, 409-414. | 1.2 | 123 |

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|---|---|---|---|
| 19 | Direct-Space Corrections Enable Fast and Accurate Lorentzâ€“Berthelot Combination Rule Lennard-Jones Lattice Summation. Journal of Chemical Theory and Computation, 2015, 11, 5737-5746. | 2.3 | 112 |
| 20 | Modeling Multibody Effects in Ionic Solutions with a Concentration Dependent Dielectric Permittivity. Physical Review Letters, 2006, 96, 147801. | 2.9 | 110 |
| 21 | Competing Adsorption between Hydrated Peptides and Water onto Metal Surfaces: From Electronic to Conformational Properties. Journal of the American Chemical Society, 2008, 130, 13460-13464. | 6.6 | 68 |
| 22 | Dynamics and Structure of Ln(III)âˆ’Aqua Ions: A Comparative Molecular Dynamics Study Using ab Initio Based Flexible and Polarizable Model Potentials. Journal of Physical Chemistry B, 2009, 113, 7270-7281. | 1.2 | 62 |
| 23 | 310-Helix Conformation Facilitates the Transition of a Voltage Sensor S4 Segment toward the Down State. Biophysical Journal, 2011, 100, 1446-1454. | 0.2 | 54 |
| 24 | An application of flexible constraints in Monte Carlo simulations of the isobaricâ€“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, 11133-11143. | 1.2 | 53 |
| 25 | Ion Pairing in Aqueous Electrolyte Solutions with Biologically Relevant Anions. Journal of Physical Chemistry B, 2011, 115, 3734-3739. | 1.2 | 46 |
| 26 | GROMACSâ€”the road ahead. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 710-715. | 6.2 | 43 |
| 27 | Molecular origin of contact line friction in dynamic wetting. Physical Review Fluids, 2018, 3, . | 1.0 | 40 |
| 28 | Fast-Growth Thermodynamic Integration:â€‰ Calculating Excess Chemical Potentials of Additive Molecules in Polymer Microstructures. Macromolecules, 2008, 41, 2283-2289. | 2.2 | 34 |
| 29 | 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. | 1.2 | 31 |
| 30 | Sequence dependency of canonical base pair opening in the DNA double helix. PLoS Computational Biology, 2017, 13, e1005463. | 1.5 | 31 |
| 31 | Algorithm improvements for molecular dynamics simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 93-108. | 6.2 | 30 |
| 32 | Driving Forces for Adsorption of Amphiphilic Peptides to the Airâˆ’Water Interface. Journal of Physical Chemistry B, 2010, 114, 11093-11101. | 1.2 | 28 |
| 33 | Further investigation on the validity of Stokesâ€“Einstein behaviour at the molecular level. Chemical Physics Letters, 2001, 334, 337-342. | 1.2 | 27 |
| 34 | Ten simple rules on how to create open access and reproducible molecular simulations of biological systems. PLoS Computational Biology, 2019, 15, e1006649. | 1.5 | 25 |
| 35 | Waterâ€“substrate physico-chemistry in wetting dynamics. Journal of Fluid Mechanics, 2015, 781, 695-711. | 1.4 | 23 |
| 36 | Modeling Solubilities of Additives in Polymer Microstructures: Single-Step Perturbation Method Based on a Soft-Cavity Reference State. Macromolecules, 2008, 41, 5055-5061. | 2.2 | 22 |

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|---|---|---|---|
| 37 | Riemann metric approach to optimal sampling of multidimensional free-energy landscapes. Physical Review E, 2018, 98, 023312. | 0.8 | 18 |
| 38 | Predictive Modeling of Phenol Chemical Potentials in Molten Bisphenol Aâ˜Polycarbonate over a Broad Temperature Range. Macromolecules, 2008, 41, 7281-7283. | 2.2 | 16 |
| 39 | The accelerated weight histogram method for alchemical free energy calculations. Journal of Chemical Physics, 2021, 154, 204103. | 1.2 | 15 |
| 40 | 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, 106-112. | 1.5 | 11 |
| 41 | Regularizing the fast multipole method for use in molecular simulation. Journal of Chemical Physics, 2019, 151, 234113. | 1.2 | 10 |
| 42 | Nanoscale sheared droplet: volume-of-fluid, phase-field and no-slip molecular dynamics. Journal of Fluid Mechanics, 2022, 940, . | 1.4 | 10 |
| 43 | Stability of Hydrophobically Modified Poly(p-phenylenesulfonate) Bundles As Observed by Molecular Dynamics Simulation. Macromolecules, 2007, 40, 1703-1707. | 2.2 | 9 |
| 44 | Chain packing in polycarbonate glasses. Journal of Chemical Physics, 2010, 132, 104901. | 1.2 | 6 |
| 45 | Interaction of Water with N,Nâ€²â˜1,2-Ethanediyl-bis(6-hydroxy-hexanamide) Crystals: A Simulation Study. Journal of Physical Chemistry B, 2009, 113, 627-631. | 1.2 | 3 |
| 46 | Electrowetting diminishes contact line friction in molecular wetting. Physical Review Fluids, 2020, 5, . | 1.0 | 3 |