

Helmut GrubmÃ¼ller

List of Publications by Year in descending order

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154
papers

16,822
citations

26630

56
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17105

122
g-index

176
all docs

176
docs citations

176
times ranked

18600
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | CHARMM36m: an improved force field for folded and intrinsically disordered proteins. <i>Nature Methods</i> , 2017, 14, 71-73. | 19.0 | 3,959 |
| 2 | Molecular Anatomy of a Trafficking Organelle. <i>Cell</i> , 2006, 127, 831-846. | 28.9 | 1,985 |
| 3 | Recognition Dynamics Up to Microseconds Revealed from an RDC-Derived Ubiquitin Ensemble in Solution. <i>Science</i> , 2008, 320, 1471-1475. | 12.6 | 963 |
| 4 | Predicting slow structural transitions in macromolecular systems: Conformational flooding. <i>Physical Review E</i> , 1995, 52, 2893-2906. | 2.1 | 573 |
| 5 | Generalized correlation for biomolecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 1053-1061. | 2.6 | 380 |
| 6 | Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5513-5524. | 5.3 | 368 |
| 7 | More bang for your buck: Improved use of GPU nodes for GROMACS 2018. <i>Journal of Computational Chemistry</i> , 2019, 40, 2418-2431. | 3.3 | 286 |
| 8 | Kinetics, Statistics, and Energetics of Lipid Membrane Electroporation Studied by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2008, 95, 1837-1850. | 0.5 | 280 |
| 9 | The dynamics and energetics of water permeation and proton exclusion in aquaporins. <i>Current Opinion in Structural Biology</i> , 2005, 15, 176-183. | 5.7 | 263 |
| 10 | The Mechanism of Proton Exclusion in the Aquaporin-1 Water Channel. <i>Journal of Molecular Biology</i> , 2003, 333, 279-293. | 4.2 | 257 |
| 11 | Structure and mechanism of the reversible photoswitch of a fluorescent protein. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 13070-13074. | 7.1 | 253 |
| 12 | Structure and Function of Water Channels. <i>Current Opinion in Structural Biology</i> , 2002, 12, 509-515. | 5.7 | 246 |
| 13 | The 2018 biomembrane curvature and remodeling roadmap. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 343001. | 2.8 | 212 |
| 14 | Mechanically Induced Titin Kinase Activation Studied by Force-Probe Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2005, 88, 790-804. | 0.5 | 195 |
| 15 | Best bang for your buck: GPU nodes for <scp>GROMACS</scp> biomolecular simulations. <i>Journal of Computational Chemistry</i> , 2015, 36, 1990-2008. | 3.3 | 195 |
| 16 | Membrane fusion. <i>Current Opinion in Cell Biology</i> , 2002, 14, 488-495. | 5.4 | 181 |
| 17 | Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1021-1024. | 13.8 | 173 |
| 18 | Constant pH Molecular Dynamics in Explicit Solvent with $\hat{\mu}$ -Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1962-1978. | 5.3 | 163 |

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|----|--|------|-----------|
| 19 | Dynamic Force Spectroscopy of Molecular Adhesion Bonds. <i>Physical Review Letters</i> , 2000, 84, 6126-6129. | 7.8 | 152 |
| 20 | Energy barriers and driving forces in tRNA translocation through the ribosome. <i>Nature Structural and Molecular Biology</i> , 2013, 20, 1390-1396. | 8.2 | 150 |
| 21 | Caught in the Act: Visualization of SNARE-Mediated Fusion Events in Molecular Detail. <i>ChemBioChem</i> , 2011, 12, 1049-1055. | 2.6 | 134 |
| 22 | Hydrophobic mismatch sorts SNARE proteins into distinct membrane domains. <i>Nature Communications</i> , 2015, 6, 5984. | 12.8 | 130 |
| 23 | Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. <i>Journal of Molecular Biology</i> , 2001, 309, 299-313. | 4.2 | 126 |
| 24 | Full correlation analysis of conformational protein dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 1294-1312. | 2.6 | 122 |
| 25 | How SNARE molecules mediate membrane fusion: Recent insights from molecular simulations. <i>Current Opinion in Structural Biology</i> , 2012, 22, 187-196. | 5.7 | 121 |
| 26 | A refined structure of human aquaporin-1. <i>FEBS Letters</i> , 2001, 504, 206-211. | 2.8 | 120 |
| 27 | Structural Basis for Polyproline-Mediated Ribosome Stalling and Rescue by the Translation Elongation Factor EF-P. <i>Molecular Cell</i> , 2017, 68, 515-527.e6. | 9.7 | 118 |
| 28 | Mechanical Properties of the Icosahedral Shell of Southern Bean Mosaic Virus: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2009, 96, 1350-1363. | 0.5 | 117 |
| 29 | Collective Langevin dynamics of conformational motions in proteins. <i>Journal of Chemical Physics</i> , 2006, 124, 214903. | 3.0 | 114 |
| 30 | Structural Heterogeneity and Quantitative FRET Efficiency Distributions of Polyprolines through a Hybrid Atomistic Simulation and Monte Carlo Approach. <i>PLoS ONE</i> , 2011, 6, e19791. | 2.5 | 108 |
| 31 | Speeding up parallel GROMACS on high-latency networks. <i>Journal of Computational Chemistry</i> , 2007, 28, 2075-2084. | 3.3 | 107 |
| 32 | A combined cryo-EM and molecular dynamics approach reveals the mechanism of ErmBL-mediated translation arrest. <i>Nature Communications</i> , 2016, 7, 12026. | 12.8 | 103 |
| 33 | Expansion of the fusion stalk and its implication for biological membrane fusion. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 11043-11048. | 7.1 | 99 |
| 34 | Chromophore Protonation State Controls Photoswitching of the Fluoroprotein asFP595. <i>PLoS Computational Biology</i> , 2008, 4, e1000034. | 3.2 | 98 |
| 35 | Photoswitching of the Fluorescent Protein asFP595: Mechanism, Proton Pathways, and Absorption Spectra. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 530-536. | 13.8 | 95 |
| 36 | Heterogeneous and rate-dependent streptavidin-biotin unbinding revealed by high-speed force spectroscopy and atomistic simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 6594-6601. | 7.1 | 95 |

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|----|---|------|-----------|
| 37 | The pathway to GTPase activation of elongation factor SelB on the ribosome. <i>Nature</i> , 2016, 540, 80-85. | 27.8 | 93 |
| 38 | Dynamics and Energetics of Permeation Through Aquaporins. What Do We Learn from Molecular Dynamics Simulations?. <i>Handbook of Experimental Pharmacology</i> , 2009, , 57-76. | 1.8 | 92 |
| 39 | Water Permeation through Gramicidin A: Desformylation and the Double Helix: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2002, 82, 2934-2942. | 0.5 | 89 |
| 40 | Quantitative Structural Analysis of Importin- β Flexibility: Paradigm for Solenoid Protein Structures. <i>Structure</i> , 2010, 18, 1171-1183. | 3.3 | 89 |
| 41 | Exploring Protein Dynamics Space: The Dynasome as the Missing Link between Protein Structure and Function. <i>PLoS ONE</i> , 2012, 7, e33931. | 2.5 | 83 |
| 42 | Automated cryo-EM structure refinement using correlation-driven molecular dynamics. <i>ELife</i> , 2019, 8, . | 6.0 | 83 |
| 43 | Accuracy and convergence of free energy differences calculated from nonequilibrium switching processes. <i>Journal of Computational Chemistry</i> , 2009, 30, 447-456. | 3.3 | 81 |
| 44 | Urea Impedes the Hydrophobic Collapse of Partially Unfolded Proteins. <i>Biophysical Journal</i> , 2009, 96, 3744-3752. | 0.5 | 69 |
| 45 | Determining equilibrium constants for dimerization reactions from molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2011, 32, 1919-1928. | 3.3 | 69 |
| 46 | A GPU-Accelerated Fast Multipole Method for GROMACS: Performance and Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6938-6949. | 5.3 | 68 |
| 47 | Kinase-activity-independent functions of atypical protein kinase C in <i>Drosophila</i> . <i>Journal of Cell Science</i> , 2009, 122, 3759-3771. | 2.0 | 67 |
| 48 | Mechanical Coupling via the Membrane Fusion SNARE Protein Syntaxin 1A: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2003, 84, 1527-1547. | 0.5 | 66 |
| 49 | An Unusual Hydrophobic Core Confers Extreme Flexibility to HEAT Repeat Proteins. <i>Biophysical Journal</i> , 2010, 99, 1596-1603. | 0.5 | 66 |
| 50 | Polar or Apolar? The Role of Polarity for Urea-Induced Protein Denaturation. <i>PLoS Computational Biology</i> , 2008, 4, e1000221. | 3.2 | 65 |
| 51 | Molecular Basis of the Light-driven Switching of the Photochromic Fluorescent Protein Padron. <i>Journal of Biological Chemistry</i> , 2010, 285, 14603-14609. | 3.4 | 65 |
| 52 | Structural basis for cooperativity of CRM1 export complex formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 960-965. | 7.1 | 64 |
| 53 | Predicting unimolecular chemical reactions: Chemical flooding. <i>Journal of Chemical Physics</i> , 2002, 116, 897-905. | 3.0 | 63 |
| 54 | Flooding in GROMACS: Accelerated barrier crossings in molecular dynamics. <i>Journal of Computational Chemistry</i> , 2006, 27, 1693-1702. | 3.3 | 63 |

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|----|---|------|-----------|
| 55 | Engineering fatty acid synthases for directed polyketide production. <i>Nature Chemical Biology</i> , 2017, 13, 363-365. | 8.0 | 63 |
| 56 | Line-Tension Controlled Mechanism for Influenza Fusion. <i>PLoS ONE</i> , 2012, 7, e38302. | 2.5 | 63 |
| 57 | Maximum likelihood trajectories from single molecule fluorescence resonance energy transfer experiments. <i>Journal of Chemical Physics</i> , 2003, 119, 9920-9924. | 3.0 | 62 |
| 58 | do_x3dna: a tool to analyze structural fluctuations of dsDNA or dsRNA from molecular dynamics simulations. <i>Bioinformatics</i> , 2015, 31, 2583-2585. | 4.1 | 59 |
| 59 | Estimating Absolute Configurational Entropies of Macromolecules: The Minimally Coupled Subspace Approach. <i>PLoS ONE</i> , 2010, 5, e9179. | 2.5 | 57 |
| 60 | Anomalous Surface Diffusion of Protons on Lipid Membranes. <i>Biophysical Journal</i> , 2014, 107, 76-87. | 0.5 | 55 |
| 61 | SESCA: Predicting Circular Dichroism Spectra from Protein Molecular Structures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5087-5102. | 5.3 | 54 |
| 62 | The Structure of the Aquaporin-1 Water Channel: A Comparison between Cryo-electron Microscopy and X-ray Crystallography. <i>Journal of Molecular Biology</i> , 2003, 325, 485-493. | 4.2 | 51 |
| 63 | Importin- β : Structural and Dynamic Determinants of a Molecular Spring. <i>Structure</i> , 2008, 16, 906-915. | 3.3 | 49 |
| 64 | Proteins in the gas phase. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 408-425. | 14.6 | 49 |
| 65 | Elastic Properties of Photoswitchable Azobenzene Polymers from Molecular Dynamics Simulations. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 2232-2237. | 13.8 | 46 |
| 66 | Torsional elasticity and energetics of F ₁ -ATPase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 7408-7413. | 7.1 | 46 |
| 67 | AMBER-DYES: Characterization of Charge Fluctuations and Force Field Parameterization of Fluorescent Dyes for Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5505-5512. | 5.3 | 44 |
| 68 | Charge-Neutral Constant pH Molecular Dynamics Simulations Using a Parsimonious Proton Buffer. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1040-1051. | 5.3 | 44 |
| 69 | Estimation of absolute solvent and solvation shell entropies via permutation reduction. <i>Journal of Chemical Physics</i> , 2007, 126, 014102. | 3.0 | 43 |
| 70 | Structural and mechanistic basis for translation inhibition by macrolide and ketolide antibiotics. <i>Nature Communications</i> , 2021, 12, 4466. | 12.8 | 43 |
| 71 | Keep It Flexible: Driving Macromolecular Rotary Motions in Atomistic Simulations with GROMACS. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1381-1393. | 5.3 | 42 |
| 72 | Quantitative Assessment of Protein Interaction with Methyl-Lysine Analogues by Hybrid Computational and Experimental Approaches. <i>ACS Chemical Biology</i> , 2012, 7, 150-154. | 3.4 | 42 |

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|----|--|------|-----------|
| 73 | Microtubule assembly governed by tubulin allosteric gain in flexibility and lattice induced fit. <i>ELife</i> , 2018, 7, . | 6.0 | 42 |
| 74 | Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility. <i>ChemBioChem</i> , 2009, 10, 1816-1822. | 2.6 | 39 |
| 75 | Conformational Dynamics of the F1-ATPase $\hat{2}$ -Subunit: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2003, 85, 1482-1491. | 0.5 | 38 |
| 76 | Active role of elongation factor G in maintaining the mRNA reading frame during translation. <i>Science Advances</i> , 2019, 5, eaax8030. | 10.3 | 38 |
| 77 | Linear-scaling soft-core scheme for alchemical free energy calculations. <i>Journal of Computational Chemistry</i> , 2012, 33, 25-33. | 3.3 | 37 |
| 78 | g_contacts: Fast contact search in bio-molecular ensemble data. <i>Computer Physics Communications</i> , 2013, 184, 2856-2859. | 7.5 | 37 |
| 79 | GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1691-1711. | 5.4 | 37 |
| 80 | Dynamic contact network between ribosomal subunits enables rapid large-scale rotation during spontaneous translocation. <i>Nucleic Acids Research</i> , 2015, 43, 6747-6760. | 14.5 | 36 |
| 81 | The Fold of Human Aquaporin 1. <i>Journal of Molecular Biology</i> , 2000, 300, 987-994. | 4.2 | 34 |
| 82 | Structure determination from single molecule X-ray scattering with three photons per image. <i>Nature Communications</i> , 2018, 9, 2375. | 12.8 | 34 |
| 83 | Thermodynamic control of $\hat{1}$ programmed ribosomal frameshifting. <i>Nature Communications</i> , 2019, 10, 4598. | 12.8 | 34 |
| 84 | Multiple time step algorithms for molecular dynamics simulations of proteins: How good are they?. <i>Journal of Computational Chemistry</i> , 1998, 19, 1534-1552. | 3.3 | 33 |
| 85 | $\langle \text{PspF} \rangle$ -binding domain $\langle \text{PspA} \rangle_{144}$ and the $\langle \text{PspA} \rangle \cdot \langle \text{PspF} \rangle$ complex: New insights into the coiled-coil-dependent regulation of $\langle \text{AAA} \rangle$ + proteins. <i>Molecular Microbiology</i> , 2015, 98, 743-759. | 2.5 | 33 |
| 86 | Molecular simulations of the ribosome and associated translation factors. <i>Current Opinion in Structural Biology</i> , 2018, 49, 27-35. | 5.7 | 33 |
| 87 | Spatiotemporal Resolution of Conformational Changes in Biomolecules by Combining Pulsed Electron Double Resonance Spectroscopy with Microsecond Freeze-Hyperquenching. <i>Journal of the American Chemical Society</i> , 2021, 143, 6981-6989. | 13.7 | 33 |
| 88 | Effects of cryo-EM cooling on structural ensembles. <i>Nature Communications</i> , 2022, 13, 1709. | 12.8 | 33 |
| 89 | Lipid Binding Defects and Perturbed Synaptogenic Activity of a Collybistin R290H Mutant That Causes Epilepsy and Intellectual Disability. <i>Journal of Biological Chemistry</i> , 2015, 290, 8256-8270. | 3.4 | 32 |
| 90 | Free Energy Landscape of Rim-Pore Expansion in Membrane Fusion. <i>Biophysical Journal</i> , 2014, 107, 2287-2295. | 0.5 | 30 |

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|-----|---|------|-----------|
| 91 | Fluctuations of primary ubiquitin folding intermediates in a force clamp. <i>Journal of Structural Biology</i> , 2007, 157, 557-569. | 2.8 | 28 |
| 92 | NuSol – Numerical solver for the 3D stationary nuclear Schrödinger equation. <i>Computer Physics Communications</i> , 2016, 198, 169-178. | 7.5 | 28 |
| 93 | A Highly Strained Nuclear Conformation of the Exportin Cse1p Revealed by Molecular Dynamics Simulations. <i>Structure</i> , 2006, 14, 1469-1478. | 3.3 | 27 |
| 94 | Exploiting Lipid Permutation Symmetry to Compute Membrane Remodeling Free Energies. <i>Physical Review Letters</i> , 2016, 117, 188102. | 7.8 | 27 |
| 95 | Accurate Three States Model for Amino Acids with Two Chemically Coupled Titrating Sites in Explicit Solvent Atomistic Constant pH Simulations and pK_a Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 147-160. | 5.3 | 27 |
| 96 | Time-Lagged Independent Component Analysis of Random Walks and Protein Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5766-5776. | 5.3 | 27 |
| 97 | Sharing Data from Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4093-4099. | 5.4 | 26 |
| 98 | Cationic and Anionic Impact on the Electronic Structure of Liquid Water. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3759-3764. | 4.6 | 26 |
| 99 | Molecular Dynamics Simulations of Protein G Challenge NMR-Derived Correlated Backbone Motions. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 3394-3399. | 13.8 | 25 |
| 100 | Primary Changes of the Mechanical Properties of Southern Bean Mosaic Virus upon Calcium Removal. <i>Biophysical Journal</i> , 2010, 98, 687-695. | 0.5 | 25 |
| 101 | A Force Buffer – Protecting Immunoglobulin Titin. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 3528-3531. | 13.8 | 23 |
| 102 | MD Simulations and FRET Reveal an Environment-Sensitive Conformational Plasticity of Importin- β . <i>Biophysical Journal</i> , 2015, 109, 277-286. | 0.5 | 23 |
| 103 | Mechanochemical Energy Transduction during the Main Rotary Step in the Synthesis Cycle of F_1 -ATPase. <i>Journal of the American Chemical Society</i> , 2017, 139, 4025-4034. | 13.7 | 23 |
| 104 | Adaptive anisotropic kernels for nonparametric estimation of absolute configurational entropies in high-dimensional configuration spaces. <i>Physical Review E</i> , 2009, 80, 011913. | 2.1 | 21 |
| 105 | Elastic Properties and Heterogeneous Stiffness of the Phi29 Motor Connector Channel. <i>Biophysical Journal</i> , 2014, 106, 1338-1348. | 0.5 | 21 |
| 106 | Towards computational specificity screening of DNA-binding proteins. <i>Nucleic Acids Research</i> , 2011, 39, 8281-8290. | 14.5 | 20 |
| 107 | TatBC-Independent TatA/Tat Substrate Interactions Contribute to Transport Efficiency. <i>PLoS ONE</i> , 2015, 10, e0119761. | 2.5 | 20 |
| 108 | Choice of fluorophore affects dynamic DNA nanostructures. <i>Nucleic Acids Research</i> , 2021, 49, 4186-4195. | 14.5 | 20 |

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|-----|--|------|-----------|
| 109 | Tight docking of membranes before fusion represents a metastable state with unique properties. <i>Nature Communications</i> , 2021, 12, 3606. | 12.8 | 20 |
| 110 | tRNA Dissociation from EF-Tu after GTP Hydrolysis: Primary Steps and Antibiotic Inhibition. <i>Biophysical Journal</i> , 2020, 118, 151-161. | 0.5 | 19 |
| 111 | ATP-Magnesium Coordination: Protein Structure-Based Force Field Evaluation and Corrections. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1922-1930. | 5.3 | 19 |
| 112 | The Low Barrier Hydrogen Bond in the Photoactive Yellow Protein: A Vacuum Artifact Absent in the Crystal and Solution. <i>Journal of the American Chemical Society</i> , 2016, 138, 16620-16631. | 13.7 | 18 |
| 113 | Velocity-Dependent Mechanical Unfolding of Bacteriorhodopsin Is Governed by a Dynamic Interaction Network. <i>Biophysical Journal</i> , 2011, 100, 1109-1119. | 0.5 | 17 |
| 114 | Structural Determinants and Mechanism of Mammalian CRM1 Allostery. <i>Structure</i> , 2013, 21, 1350-1360. | 3.3 | 17 |
| 115 | Transient Secondary and Tertiary Structure Formation Kinetics in the Intrinsically Disordered State of λ -Synuclein from Atomistic Simulations. <i>ChemPhysChem</i> , 2018, 19, 2507-2511. | 2.1 | 17 |
| 116 | How proteins open fusion pores: insights from molecular simulations. <i>European Biophysics Journal</i> , 2021, 50, 279-293. | 2.2 | 17 |
| 117 | Force Distribution Analysis of Mechanochemically Reactive Dimethylcyclobutene. <i>ChemPhysChem</i> , 2013, 14, 2687-2697. | 2.1 | 15 |
| 118 | Computing Spatially Resolved Rotational Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 108-118. | 5.3 | 15 |
| 119 | Microtubule instability driven by longitudinal and lateral strain propagation. <i>PLoS Computational Biology</i> , 2020, 16, e1008132. | 3.2 | 15 |
| 120 | Determining Free-Energy Differences Through Variationally Derived Intermediates. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3504-3512. | 5.3 | 15 |
| 121 | Probing the Accuracy of Explicit Solvent Constant pH Molecular Dynamics Simulations for Peptides. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2561-2569. | 5.3 | 13 |
| 122 | Per Mut: Spatially Resolved Hydration Entropies from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2090-2098. | 5.3 | 13 |
| 123 | Universal Relaxation Governs the Nonequilibrium Elasticity of Biomolecules. <i>Physical Review Letters</i> , 2012, 109, 118304. | 7.8 | 12 |
| 124 | Bayesian orientation estimate and structure information from sparse single-molecule x-ray diffraction images. <i>Physical Review E</i> , 2014, 90, 022714. | 2.1 | 12 |
| 125 | What happens if the room at the bottom runs out? A close look at small water pores. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 7421-7422. | 7.1 | 10 |
| 126 | Binding Affinities Controlled by Shifting Conformational Equilibria: Opportunities and Limitations. <i>Biophysical Journal</i> , 2015, 108, 2585-2590. | 0.5 | 10 |

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|-----|--|------|-----------|
| 127 | Phi29 Connector-DNA Interactions Govern DNA Crunching and Rotation, Supporting the Check-Valve Model. <i>Biophysical Journal</i> , 2016, 110, 455-469. | 0.5 | 10 |
| 128 | How accurate is circular dichroism-based model validation?. <i>European Biophysics Journal</i> , 2020, 49, 497-510. | 2.2 | 10 |
| 129 | Spatially resolved free-energy contributions of native fold and molten-globule-like Crambin. <i>Biophysical Journal</i> , 2021, 120, 3470-3482. | 0.5 | 10 |
| 130 | Intersubunit Coupling Enables Fast CO ₂ -Fixation by Reductive Carboxylases. <i>ACS Central Science</i> , 2022, 8, 1091-1101. | 11.3 | 10 |
| 131 | Sequential Water and Headgroup Merger: Membrane Poration Paths and Energetics from MD Simulations. <i>Biophysical Journal</i> , 2020, 119, 2418-2430. | 0.5 | 8 |
| 132 | Folding of VemP into translation-arresting secondary structure is driven by the ribosome exit tunnel. <i>Nucleic Acids Research</i> , 2022, 50, 2258-2269. | 14.5 | 8 |
| 133 | Molecular Determinants of Snurportin 1 Ligand Affinity and Structural Response upon Binding. <i>Biophysical Journal</i> , 2009, 97, 581-589. | 0.5 | 7 |
| 134 | GROMACS implementation of free energy calculations with non-pairwise Variationally derived Intermediates. <i>Computer Physics Communications</i> , 2021, 264, 107931. | 7.5 | 7 |
| 135 | Bending-torsional elasticity and energetics of the plus-end microtubule tip. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2115516119. | 7.1 | 7 |
| 136 | Implementation of a Bayesian secondary structure estimation method for the SESCA circular dichroism analysis package. <i>Computer Physics Communications</i> , 2021, 266, 108022. | 7.5 | 6 |
| 137 | Estimating ruggedness of free-energy landscapes of small globular proteins from principal component analysis of molecular dynamics trajectories. <i>Physical Review E</i> , 2022, 105, 044404. | 2.1 | 6 |
| 138 | Kraftspektroskopie von einzelnen Biomolekülen: Biologische Makromoleküle besser begreifen mit Einzelmolekülkraftmessungen und Computersimulationen. <i>Physik Journal</i> , 2001, 57, 55-61. | 0.1 | 4 |
| 139 | Estimating the Orientational Entropy of Water at Protein Interfaces. <i>Biophysical Journal</i> , 2011, 100, 613a. | 0.5 | 4 |
| 140 | A Quantitative Model for cAMP Binding to the Binding Domain of MloK1. <i>Biophysical Journal</i> , 2016, 111, 1668-1678. | 0.5 | 4 |
| 141 | Variationally derived intermediates for correlated free-energy estimates between intermediate states. <i>Physical Review E</i> , 2020, 102, 043312. | 2.1 | 3 |
| 142 | A CUDA fast multipole method with highly efficient M2L far field evaluation. <i>International Journal of High Performance Computing Applications</i> , 2021, 35, 97-117. | 3.7 | 3 |
| 143 | BASDet: Bayesian approach(es) for structure determination from single molecule X-ray diffraction images. <i>Computer Physics Communications</i> , 2016, 201, 159-166. | 7.5 | 2 |
| 144 | GROMEX: A Scalable and Versatile Fast Multipole Method for Biomolecular Simulation. <i>Lecture Notes in Computational Science and Engineering</i> , 2020, , 517-543. | 0.3 | 2 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|------|-----------|
| 145 | Small-sample limit of the Bennett acceptance ratio method and the variationally derived intermediates. Physical Review E, 2021, 104, 054133. | 2.1 | 2 |
| 146 | Inside Cover: Primary Steps of pH-Dependent Insulin Aggregation Kinetics are Governed by Conformational Flexibility (ChemBioChem 11/2009). ChemBioChem, 2009, 10, 1742-1742. | 2.6 | 1 |
| 147 | Cover Picture: Multistep Binding of Divalent Cations to Phospholipid Bilayers: A Molecular Dynamics Study (Angew. Chem. Int. Ed. 8/2004). Angewandte Chemie - International Edition, 2004, 43, 911-911. | 13.8 | 0 |
| 148 | Atomistic Simulations of the Human Proteasome Inhibited by a Covalent Ligand. , 2021, , 47-57. | | 0 |
| 149 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |
| 150 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |
| 151 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |
| 152 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |
| 153 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |
| 154 | Microtubule instability driven by longitudinal and lateral strain propagation. , 2020, 16, e1008132. | | 0 |