# Ulrich KleinekathÃ¶fer

List of Publications by Year
in descending order



| 176 | 5,635 | 87723 38 | 98622 67 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 181 | 181 | 181 | 4340 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Group three nitride clusters as promising components for nanoelectronics. Materials Today Chemistry, 2022, 23, 100751. | 1.7 | 2 |
| 2 | Coherent and Incoherent Contributions to Molecular Electron Transport. Journal of Chemical Physics, 2022, 156, 094302. | 1.2 | 12 |
| 3 | Permeation of Fosfomycin through the Phosphate-Specific Channels OprP and OprO of Pseudomonas aeruginosa. Journal of Physical Chemistry B, 2022, 126, 1388-1403. | 1.2 | 7 |
| 4 | Transverse electronic transport through nucleobase-pairs of a DNA wire. Materials Today Chemistry, 2022, 24, 100834. | 1.7 | 2 |
| 5 | Changes in Salt Concentration Modify the Translocation of Neutral Molecules through a Î”CymA Nanopore in a Non-monotonic Manner. ACS Nano, 2022, 16, 7701-7712. | 7.3 | 6 |
| 6 | Spectral densities and absorption spectra of the core antenna complex CP43 from photosystem II. Journal of Chemical Physics, 2022, 156, . | 1.2 | 8 |
| 7 | Permeation eines 5.1â€kDaâ€Peptides durch einen Proteinkanal: Molekulare Basis der Translokation von Protamin durch CymA aus Klebsiella Oxytoca **. Angewandte Chemie, 2021, 133, 8170-8175. | 1.6 | 2 |
| 8 | How to Enter a Bacterium: Bacterial Porins and the Permeation of Antibiotics. Chemical Reviews, 2021, 121, 5158-5192. | 23.0 | 103 |
| 9 | Largeâ€Peptide Permeation Through a Membrane Channel: Understanding Protamine Translocation Through CymA from Klebsiella Oxytoca**. Angewandte Chemie - International Edition, 2021, 60, 8089-8094. | 7.2 | 15 |
| 10 | Improved Sampling and Free Energy Estimates for Antibiotic Permeation through Bacterial Porins. Journal of Chemical Theory and Computation, 2021, 17, 4564-4577. | 2.3 | 15 |
| 11 | Time-dependent atomistic simulations of the CP29 light-harvesting complex. Journal of Chemical Physics, 2021, 155, 055103. | 1.2 | 10 |
| 12 | Robust Strategy for Photoprotection in the Light-Harvesting Antenna of Diatoms: A Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2021, 12, 9626-9633. | 2.1 | 12 |
| 13 | Multiscale QM/MM molecular dynamics simulations of the trimeric major light-harvesting complex II. Physical Chemistry Chemical Physics, 2021, 23, 7407-7417. | 1.3 | 24 |
| 14 | Millisecond-Long Simulations of Antibiotics Transport through Outer Membrane Channels. Journal of Chemical Theory and Computation, 2021, 17, 549-559. | 2.3 | 8 |
| 15 | DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667. | 2.1 | 34 |
| 16 | Voltage-Dependent Transport of Neutral Solutes through Nanopores: A Molecular View. Journal of Physical Chemistry B, 2020, 124, 10718-10731. | 1.2 | 8 |
| 17 | The structure of the antimicrobial human cathelicidin LL-37 shows oligomerization and channel formation in the presence of membrane mimics. Scientific Reports, 2020, 10, 17356. | 1.6 | 54 |
| 18 | Dynamic interaction of fluoroquinolones with magnesium ions monitored using bacterial outer membrane nanopores. Chemical Science, 2020, 11, 10344-10353. | 3.7 | 23 |

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| 19 | Structural and functional insights into oligopeptide acquisition by the RagAB transporter from Porphyromonas gingivalis. Nature Microbiology, 2020, 5, 1016-1025. | 5.9 | 46 |
| 20 | Computational Modeling of Ion Transport in Bulk and through a Nanopore Using the Drude Polarizable Force Field. Journal of Chemical Information and Modeling, 2020, 60, 3188-3203. | 2.5 | 16 |
| 21 | Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 2591-2604. | 2.5 | 24 |
| 22 | Quantum biology revisited. Science Advances, 2020, 6, eaaz4888. | 4.7 | 266 |
| 23 | Exploration of Free Energy Surfaces Across a Membrane Channel Using Metadynamics and Umbrella Sampling. Journal of Chemical Theory and Computation, 2020, 16, 2751-2765. | 2.3 | 26 |
| 24 | Benchmark and performance of long-range corrected time-dependent density functional tight binding (LC-TD-DFTB) on rhodopsins and light-harvesting complexes. Physical Chemistry Chemical Physics, 2020, 22, 10500-10518. | 1.3 | 36 |
| 25 | On a chlorophyll-caroteinoid coupling in LHCII. Chemical Physics, 2019, 526, 110439. | 0.9 | 24 |
| 26 | Structural Basis for Allosteric Regulation in the Major Antenna Trimer of Photosystem II. Journal of Physical Chemistry B, 2019, 123, 9609-9615. | 1.2 | 17 |
| 27 | Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23. | 13.5 | 122 |
| 28 | Fosfomycin Permeation through the Outer Membrane Porin OmpF. Biophysical Journal, 2019, 116, 258-269. | 0.2 | 24 |
| 29 | Fine tuning of the photosystem II major antenna mobility within the thylakoid membrane of higher plants. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 183059. | 1.4 | 30 |
| 30 | Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. Journal of Physical Chemistry B, 2019, 123, 5700-5708. | 1.2 | 11 |
| 31 | Chebyshev hierarchical equations of motion for systems with arbitrary spectral densities and temperatures. Journal of Chemical Physics, 2019, 150, 244104. | 1.2 | 29 |
| 32 | Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. Journal of Physical Chemistry B, 2019, 123, 4625-4635. | 1.2 | 18 |
| 33 | Dephasing in a Molecular Junction Viewed from a Time-Dependent and a Time-Independent Perspective. Journal of Physical Chemistry C, 2019, 123, 9590-9599. | 1.5 | 5 |
| 34 | A Multidisciplinary Approach toward Identification of Antibiotic Scaffolds for Acinetobacter baumannii. Structure, 2019, 27, 268-280.e6. | 1.6 | 41 |
| 35 | Structural basis for chitin acquisition by marine Vibrio species. Nature Communications, 2018, 9, 220. | 5.8 | 37 |
| 36 | Water-mediated interactions enable smooth substrate transport in a bacterial efflux pump. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 836-845. | 1.1 | 42 |

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| 37 | Enrofloxacin Permeation Pathways across the Porin OmpC. Journal of Physical Chemistry B, 2018, 122, 1417-1426. | 1.2 | 24 |
| 38 | Understanding the Structure and Function of the DcaP Channel from Acinetobacter baumannii using MD Simulations. Biophysical Journal, 2018, 114, 491a. | 0.2 | 0 |
| 39 | Brownian Dynamics Approach Including Explicit Atoms for Studying Ion Permeation and Substrate Translocation across Nanopores. Journal of Chemical Theory and Computation, 2018, 14, 6701-6713. | 2.3 | 11 |
| 40 | Non-equilibrium Greenâ€™s function transport theory for molecular junctions with general molecule-lead coupling and temperatures. Journal of Chemical Physics, 2018, 149, 234108. | 1.2 | 12 |
| 41 | Simulation Study of Occk5 Functional Properties in Pseudomonas aeruginosa Outer Membranes. Journal of Physical Chemistry B, 2018, 122, 8185-8192. | 1.2 | 12 |
| 42 | Identification and characterization of smallest pore-forming protein in the cell wall of pathogenic Corynebacterium urealyticum DSM 7109. BMC Biochemistry, 2018, 19, 3. | 4.4 | 7 |
| 43 | Environmental effects on the dynamics in the light-harvesting complexes LH2 and LH3 based on molecular simulations. Chemical Physics, 2018, 515, 141-151. | 0.9 | 16 |
| 44 | Microsecond Simulation of Electron Transfer in DNA: Bottom-Up Parametrization of an Efficient Electron Transfer Model Based on Atomistic Details. Journal of Physical Chemistry B, 2017, 121, 529-549. | 1.2 | 23 |
| 45 | Structural basis for nutrient acquisition by dominant members of the human gut microbiota. Nature, 2017, 541, 407-411. | 13.7 | 188 |
| 46 | Impact of Electronic Fluctuations and Their Description on the Exciton Dynamics in the Light-Harvesting Complex PE545. Journal of Physical Chemistry B, 2017, 121, 1330-1339. | 1.2 | 26 |
| 47 | Single Residue Acts as Gate in OccK Channels. Journal of Physical Chemistry B, 2017, 121, 2614-2621. | 1.2 | 15 |
| 48 | Dephasing Times in the Phycobiliprotein Antenna Complexes PE545 and PE555. Biophysical Journal, 2017, 112, 442a. | 0.2 | 0 |
| 49 | Tsx as a Nucleoside Channel. Biophysical Journal, 2017, 112, 450a. | 0.2 | 0 |
| 50 | Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. Journal of Chemical Theory and Computation, 2017, 13, 286-296. | 2.3 | 16 |
| 51 | Structural basis for maintenance of bacterial outer membrane lipid asymmetry. Nature Microbiology, 2017, 2, 1616-1623. | 5.9 | 118 |
| 52 | Conversion of OprO into an OprP-like Channel by Exchanging Key Residues in the Channel Constriction. Biophysical Journal, 2017, 113, 829-834. | 0.2 | 10 |
| 53 | Characterization of Ciprofloxacin Permeation Pathways across the Porin OmpC Using Metadynamics and a String Method. Journal of Chemical Theory and Computation, 2017, 13, 4553-4566. | 2.3 | 41 |
| 54 | Relation between Vibrational Dephasing Time and Energy Gap Fluctuations. Journal of Physical Chemistry B, 2017, 121, 6471-6478. | 1.2 | 5 |

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| 55 | Protein Arrangement Effects on the Exciton Dynamics in the PE555 Complex. Journal of Physical Chemistry B, 2017, 121, 3228-3236. | 1.2 | 13 |
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| 60 | Chebyshev Expansion Applied to Dissipative Quantum Systems. Journal of Physical Chemistry A, 2016, 120, 3270-3277. | 1.1 | 16 |
| 61 | Role of Electroosmosis in the Permeation of Neutral Molecules: CymA and Cyclodextrin as an Example. Biophysical Journal, 2016, 110, 600-611. | 0.2 | 55 |
| 62 | Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems. Journal of Physical Chemistry Letters, 2016, 7, 1102-1108. | 2.1 | 10 |
| 63 | Environmental Coupling and Population Dynamics in the PE545 Light-Harvesting Complex. Biophysical Journal, 2015, 108, 604a-605a. | 0.2 | 0 |
| 64 | Computational Study of Correlated Domain Motions in the AcrB Efflux Transporter. BioMed Research International, 2015, 2015, 1-12. | 0.9 | 14 |
| 65 | Theoretical analysis of ion conductance and gating transitions in the OpdK (OccK1) channel. Analyst, The, 2015, 140, 4855-4864. | 1.7 | 12 |
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| 67 | AcrB drug-binding pocket substitution confers clinically relevant resistance and altered substrate specificity. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3511-3516. | 3.3 | 165 |
| 68 | Influence of Force Fields and Quantum Chemistry Approach on Spectral Densities of BChl a in Solution and in FMO Proteins. Journal of Physical Chemistry B, 2015, 119, 9995-10004. | 1.2 | 82 |
| 69 | Outer-membrane translocation of bulky small molecules by passive diffusion. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2991-9. | 3.3 | 70 |
| 70 | Understanding the Translocation of Fluoroquinolones through OmpC using the Metadynamics. Biophysical Journal, 2015, 108, 443a. | 0.2 | 0 |
| 71 | Using the Chebychev expansion in quantum transport calculations. Journal of Chemical Physics, 2015, 142, 154103. | 1.2 | 16 |
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| 74 | OmpW of Caulobacter crescentus Functions as an Outer Membrane Channel for Cations. PLoS ONE, 2015, 10, e0143557. | 1.1 | 18 |
| 75 | Different Types of Vibrations Interacting with Electronic Excitations in Phycoerythrin 545 and Fennaâ€“Matthewsâ€“Olson Antenna Systems. Journal of Physical Chemistry Letters, 2014, 5, 3131-3137. | 2.1 | 51 |
| 76 | Environmental Effects in the FMO and PE545 Photosynthetic Complexes. Biophysical Journal, 2014, 106, 181a-182a. | 0.2 | 0 |
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| 78 | Role of the Central Arginine R133 toward the Ion Selectivity of the Phosphate Specific Channel OprP: Effects of Charge and Solvation. Biochemistry, 2013, 52, 5522-5532. | 1.2 | 27 |
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| 82 | Simulation of Ion Transport through an N-Acetylneuraminic Acid-Inducible Membrane Channel: From Understanding to Engineering. Journal of Physical Chemistry B, 2013, 117, 15966-15975. | 1.2 | 7 |
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| 85 | Juxtaposing density matrix and classical path-based wave packet dynamics. Journal of Chemical Physics, 2012, 136, 214101. | 1.2 | 38 |
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| 87 | Modeling the Ion Selectivity of the Phosphate Specific Channel OprP. Journal of Physical Chemistry Letters, 2012, 3, 3639-3645. | 2.1 | 28 |
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| 89 | Preparational Effects on the Excitation Energy Transfer in the FMO Complex. Journal of Physical Chemistry B, 2012, 116, 3900-3906. | 1.2 | 19 |
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| 97 | Role of Water during the Extrusion of Substrates by the Efflux Transporter AcrB. Journal of Physical Chemistry B, 2011, 115, 8278-8287. | 1.2 | 38 |
| 98 | Probing the Transport of Ionic Liquids in Aqueous Solution through Nanopores. Journal of Physical Chemistry Letters, 2011, 2, 2331-2336. | 2.1 | 29 |
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| 101 | DNA condensation by TmHU studied by optical tweezers, AFM and molecular dynamics simulations. Journal of Biological Physics, 2011, 37, 117-131. | 0.7 | 7 |
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| 110 | Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. Biophysical Journal, 2010, 98, 628a. | 0.2 | 1 |
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| 121 | Ion Transport through OmpF in Molecular Dynamics Simulations and Experiments. Biophysical Journal, 2009, 96, 661a. | 0.2 | 0 |
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