Ulrich KleinekathÃ¶fer

List of Publications by Year
in descending order

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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	Quantum biology revisited. Science Advances, 2020, 6, eaaz4888.	4.7	266
2	Excitons in a photosynthetic light-harvesting system: A combined molecular dynamics, quantum chemistry, and polaron model study. Physical Review E, 2002, 65, 031919.	0.8	261
3	From Atomistic Modeling to Excitation Transfer and Two-Dimensional Spectra of the FMO Light-Harvesting Complex. Journal of Physical Chemistry B, 2011, 115, 8609-8621.	1.2	197
4	Theory and Simulation of the Environmental Effects on FMO Electronic Transitions. Journal of Physical Chemistry Letters, 2011, 2, 1771-1776.	2.1	193
5	Structural basis for nutrient acquisition by dominant members of the human gut microbiota. Nature, 2017, 541, 407-411.	13.7	188
6	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
7	Time-Dependent Atomistic View on the Electronic Relaxation in Light-Harvesting System II. Journal of Physical Chemistry B, 2010, 114, 12427-12437.	1.2	140
8	Quest for Spatially Correlated Fluctuations in the FMO Light-Harvesting Complex. Journal of Physical Chemistry B, 2011, 115, 758-764.	1.2	128
9	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
10	The influence of ultrafast laser pulses on electron transfer in molecular wires studied by a non-Markovian density-matrix approach. Journal of Chemical Physics, 2006, 124, 044712.	1.2	121
11	Structural basis for maintenance of bacterial outer membrane lipid asymmetry. Nature Microbiology, 2017, 2, 1616-1623.	5.9	118
12	Non-Markovian theories based on a decomposition of the spectral density. Journal of Chemical Physics, 2004, 121, 2505.	1.2	115
13	Calculation of absorption spectra for light-harvesting systems using non-Markovian approaches as well as modified Redfield theory. Journal of Chemical Physics, 2006, 124, 084903.	1.2	104
14	How to Enter a Bacterium: Bacterial Porins and the Permeation of Antibiotics. Chemical Reviews, 2021, 121, 5158-5192.	23.0	103
15	Potentials for some rare gas and alkali-helium systems calculated from the surface integral method. Chemical Physics Letters, 1996, 249, 257-263.	1.2	95
16	Understanding Ion Conductance on a Molecular Level: An All-Atom Modeling of the Bacterial Porin OmpF. Biophysical Journal, 2009, 97, 1898-1906.	0.2	88
17	Long Range Binding in Alkali-Helium Pairs. Physical Review Letters, 1999, 83, 4717-4720.	2.9	87
18	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. PLoS Computational Biology, 2010, 6, e1000806.	1.5	83

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19	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
20	Effect of the F610A Mutation on Substrate Extrusion in the AcrB Transporter: Explanation and Rationale by Molecular Dynamics Simulations. Journal of the American Chemical Society, 2011, 133, 10704-10707.	6.6	79
21	Solvent Fluctuations Drive the Hole Transfer in DNA: A Mixed Quantumâ^'Classical Study. Journal of Physical Chemistry B, 2009, 113, 13107-13117.	1.2	71
22	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
23	Coherent laser control of the current through molecular junctions. Europhysics Letters, 2007, 79, 27006.	0.7	61
24	Transport at the nanoscale: temperature dependence of ion conductance. European Biophysics Journal, 2008, 38, 121-125.	1.2	60
25	Computational modeling of ion transport through nanopores. Nanoscale, 2012, 4, 6166.	2.8	60
26	Atomistic Modeling of Two-Dimensional Electronic Spectra and Excited-State Dynamics for a Light Harvesting 2 Complex. Journal of Physical Chemistry B, 2015, 119, 1302-1313.	1.2	59
27	Reduced dynamics of coupled harmonic and anharmonic oscillators using higher-order perturbation theory. Journal of Chemical Physics, 2007, 126, 114102.	1.2	58
28	Pulling Peptides across Nanochannels: Resolving Peptide Binding and Translocation through the Hetero-oligomeric Channel from Nocardia farcinica. ACS Nano, 2012, 6, 10699-10707.	7.3	57
29	Role of Electroosmosis in the Permeation of Neutral Molecules: CymA and Cyclodextrin as an Example. Biophysical Journal, 2016, 110, 600-611.	0.2	55
30	Comparing the Temperature-Dependent Conductance of the Two Structurally Similar E. coli Porins OmpC and OmpF. Biophysical Journal, 2010, 98, 1830-1839.	0.2	54
31	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
32	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
33	Switching the current through model molecular wires with Gaussian laser pulses. Europhysics Letters, 2006, 75, 139-145.	0.7	49
34	Structural and functional insights into oligopeptide acquisition by the RagAB transporter from Porphyromonas gingivalis. Nature Microbiology, 2020, 5, 1016-1025.	5.9	46
35	Van der Waals potentials of He2, Ne2, and Ar2 with the exchange energy calculated by the surface integral method. Journal of Chemical Physics, 1997, 107, 9502-9513.	1.2	45
36	Simulations of outer membrane channels and their permeability. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1760-1771.	1.4	44

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37	Transitions between Closed and Open Conformations of TolC: The Effects of Ions in Simulations. Biophysical Journal, 2009, 96, 3116-3125.	0.2	43
38	Boundary-condition-determined wave function for the ground state of helium and isoelectronic ions. Physical Review A, 1996, 54, 2840-2849.	1.0	42
39	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
40	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
41	A Multidisciplinary Approach toward Identification of Antibiotic Scaffolds for Acinetobacter baumannii. Structure, 2019, 27, 268-280.e6.	1.6	41
42	Structure, Dynamics, and Substrate Specificity of the OprO Porin from Pseudomonas aeruginosa. Biophysical Journal, 2015, 109, 1429-1438.	0.2	39
43	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
44	Juxtaposing density matrix and classical path-based wave packet dynamics. Journal of Chemical Physics, 2012, 136, 214101.	1.2	38
45	Structural basis for chitin acquisition by marine Vibrio species. Nature Communications, 2018, 9, 220.	5.8	37
46	Femtosecond laser pulse control of electron transfer processes. Journal of Chemical Physics, 2002, 117, 636-646.	1.2	36
47	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
48	Perturbative treatment of intercenter coupling in the framework of Redfield theory. Chemical Physics, 2001, 268, 121-130.	0.9	35
49	The FMO Complex in a Glycerolâ€“Water Mixture. Journal of Physical Chemistry B, 2013, 117, 7157-7163.	1.2	34
50	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667.	2.1	34
51	Influence of static and dynamic disorder on the anisotropy of emission in the ring antenna subunits of purple bacteria photosynthetic systems. Chemical Physics, 2002, 275, 1-13.	0.9	33
52	Efficiency of different numerical methods for solving Redfield equations. Journal of Chemical Physics, 2001, 114, 1497-1504.	1.2	32
53	Time-Dependent View of Sequential Transport through Molecules with Rapidly Fluctuating Bridges. Physical Review Letters, 2012, 109, 176802.	2.9	32
54	Ground state potentials for alkaline-earthâ€“helium diatoms calculated by the surface integral method. Chemical Physics Letters, 2000, 324, 403-410.	1.2	31

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55	Tailoring current flow patterns through molecular wires using shaped optical pulses. Physical Review B, 2008, 77, .	1.1	30
56	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
57	Probing the Transport of Ionic Liquids in Aqueous Solution through Nanopores. Journal of Physical Chemistry Letters, 2011, 2, 2331-2336.	2.1	29
58	Chebyshev hierarchical equations of motion for systems with arbitrary spectral densities and temperatures. Journal of Chemical Physics, 2019, 150, 244104.	1.2	29
59	Modeling the Ion Selectivity of the Phosphate Specific Channel OprP. Journal of Physical Chemistry Letters, 2012, 3, 3639-3645.	2.1	28
60	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
61	Modeling charge transport in DNA using multiâ€scale methods. Physica Status Solidi (B): Basic Research, 2013, 250, 2277-2287.	0.7	26
62	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
63	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
64	Exciton scattering in light-harvesting systems of purple bacteria. Journal of Luminescence, 2001, 94-95, 447-450.	1.5	24
65	Tuning the Affinity of Anion Binding Sites in Porin Channels with Negatively Charged Residues: Molecular Details for OprP. ACS Chemical Biology, 2015, 10, 441-451.	1.6	24
66	Enrofloxacin Permeation Pathways across the Porin OmpC. Journal of Physical Chemistry B, 2018, 122, 1417-1426.	1.2	24
67	On a chlorophyll-caroteinoid coupling in LHCII. Chemical Physics, 2019, 526, 110439.	0.9	24
68	Fosfomycin Permeation through the Outer Membrane Porin OmpF. Biophysical Journal, 2019, 116, 258-269.	0.2	24
69	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
70	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
71	Domain Motion of Individual F1-ATPase Î²-Subunits during Unbiased Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2011, 115, 7267-7274.	1.1	23
72	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

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73	Dynamic interaction of fluoroquinolones with magnesium ions monitored using bacterial outer membrane nanopores. Chemical Science, 2020, 11, 10344-10353.	3.7	23
74	Suppressing the current through molecular wires: comparison of two mechanisms. New Journal of Physics, 2008, 10, 085005.	1.2	22
75	Electron Transfer in Porphyrin Complexes in Different Solvents. Journal of Physical Chemistry A, 2000, 104, 5413-5421.	1.1	20
76	Stochastic unraveling of Redfield master equations and its application to electron transfer problems. Journal of Chemical Physics, 2003, 119, 6635-6646.	1.2	20
77	Treatment of timeâ€dependent effects in molecular junctions. Physica Status Solidi (B): Basic Research, 2013, 250, 2288-2297.	0.7	20
78	Preparational Effects on the Excitation Energy Transfer in the FMO Complex. Journal of Physical Chemistry B, 2012, 116, 3900-3906.	1.2	19
79	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
80	OmpW of Caulobacter crescentus Functions as an Outer Membrane Channel for Cations. PLoS ONE, 2015, 10, e0143557.	1.1	18
81	Angular momentum coupling in the exchange energy of multielectron systems. Journal of Chemical Physics, 1995, 103, 6617-6630.	1.2	17
82	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
83	Stochastic unraveling of time-local quantum master equations beyond the Lindblad class. Physical Review E, 2002, 66, 037701.	0.8	16
84	A time-dependent modified Redfield theory for absorption spectra applied to light-harvesting systems. Journal of Luminescence, 2007, 125, 126-132.	1.5	16
85	Coherent control of the spin current through a quantum dot. European Physical Journal B, 2009, 68, 103-109.	0.6	16
86	Using the Chebychev expansion in quantum transport calculations. Journal of Chemical Physics, 2015, 142, 154103.	1.2	16
87	Chebyshev Expansion Applied to Dissipative Quantum Systems. Journal of Physical Chemistry A, 2016, 120, 3270-3277.	1.1	16
88	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. Journal of Chemical Theory and Computation, 2017, 13, 286-296.	2.3	16
89	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
90	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

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91	Comparison of two models for bridge-assisted charge transfer. Journal of Luminescence, 1999, 83-84, 235-240.	1.5	15
92	A density matrix approach to photoinduced electron injection. Journal of Luminescence, 2001, 94-95, 471-474.	1.5	15
93	Memory Effects in the Fluorescence Depolarization Dynamics Studied within the B850 Ring of Purple Bacteria. Journal of Physical Chemistry B, 2003, 107, 14094-14102.	1.2	15
94	Single Residue Acts as Gate in OccK Channels. Journal of Physical Chemistry B, 2017, 121, 2614-2621.	1.2	15
95	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
96	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
97	Generalized Heitler-London theory with exchange energy by the surface integral method: an application to the alkali metal dimer cations. Chemical Physics Letters, 1996, 257, 651-657.	1.2	14
98	Computational Study of Correlated Domain Motions in the AcrB Efflux Transporter. BioMed Research International, 2015, 2015, 1-12.	0.9	14
99	BROMOCEA Code: An Improved Grand Canonical Monte Carlo/Brownian Dynamics Algorithm Including Explicit Atoms. Journal of Chemical Theory and Computation, 2016, 12, 2401-2417.	2.3	14
100	Corynebacterium jeikeium jk0268 Constitutes for the 40 Amino Acid Long PorACj, Which Forms a Homooligomeric and Anion-Selective Cell Wall Channel. PLoS ONE, 2013, 8, e75651.	1.1	14
101	Extension of the mapped Fourier method to time-dependent problems. Physical Review E, 1999, 60, 4926-4933.	0.8	13
102	The generalized Heitlerâ€“London theory for the H3 potential energy surface. Journal of Chemical Physics, 1999, 111, 3377-3386.	1.2	13
103	Coherent destruction of the current through molecular wires using short laser pulses. Physica Status Solidi (B): Basic Research, 2006, 243, 3775-3781.	0.7	13
104	Protein Arrangement Effects on the Exciton Dynamics in the PE555 Complex. Journal of Physical Chemistry B, 2017, 121, 3228-3236.	1.2	13
105	Theoretical analysis of ion conductance and gating transitions in the OpdK (OccK1) channel. Analyst, The, 2015, 140, 4855-4864.	1.7	12
106	Environmental coupling and population dynamics in the PE545 light-harvesting complex. Journal of Luminescence, 2016, 169, 406-409.	1.5	12
107	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
108	Simulation Study of Occk5 Functional Properties in Pseudomonas aeruginosa Outer Membranes. Journal of Physical Chemistry B, 2018, 122, 8185-8192.	1.2	12

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109	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
110	Coherent and Incoherent Contributions to Molecular Electron Transport. Journal of Chemical Physics, 2022, 156, 094302.	1.2	12
111	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
112	Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. Journal of Physical Chemistry B, 2019, 123, 5700-5708.	1.2	11
113	Shaping femtosecond coherent anti-Stokes Raman spectra using optimal control theory. Physical Chemistry Chemical Physics, 2008, 10, 2058.	1.3	10
114	Relation between Dephasing Time and Energy Gap Fluctuations in Biomolecular Systems. Journal of Physical Chemistry Letters, 2016, 7, 1102-1108.	2.1	10
115	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
116	Time-dependent atomistic simulations of the CP29 light-harvesting complex. Journal of Chemical Physics, 2021, 155, 055103.	1.2	10
117	Laser-driven molecular wires studied by a non-Markovian density matrix approach. Journal of Luminescence, 2006, 119-120, 462-467.	1.5	9
118	Permeation through nanochannels: revealing fast kinetics. Journal of Physics Condensed Matter, 2010, 22, 454131.	0.7	9
119	Modeling of lightâ€harvesting in purple bacteria using a timeâ€dependent Hamiltonian approach. Physica Status Solidi (B): Basic Research, 2011, 248, 393-398.	0.7	9
120	Ultrafast vibrational dynamics in higher electronic excited states of iodine. Journal of Raman Spectroscopy, 2009, 40, 822-827.	1.2	8
121	Voltage-Dependent Transport of Neutral Solutes through Nanopores: A Molecular View. Journal of Physical Chemistry B, 2020, 124, 10718-10731.	1.2	8
122	Millisecond-Long Simulations of Antibiotics Transport through Outer Membrane Channels. Journal of Chemical Theory and Computation, 2021, 17, 549-559.	2.3	8
123	Spectral densities and absorption spectra of the core antenna complex CP43 from photosystem II. Journal of Chemical Physics, 2022, 156, .	1.2	8
124	Three-body exchange energies in H3 and He3 calculated by the surface integral method. Journal of Chemical Physics, 2000, 113, 948-956.	1.2	7
125	Timeâ€dependent suppression of current through molecular junctions. Physica Status Solidi (B): Basic Research, 2008, 245, 2720-2724.	0.7	7
126	Optimal control of shot noise and Fano factor by external fields. European Physical Journal B, 2010, 76, 309-319.	0.6	7

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127	Probing the vibrational dynamics of high-lying electronic states using pump-degenerate four-wave mixing. Physical Chemistry Chemical Physics, 2010, 12, 1351-1356.	1.3	7
128	DNA condensation by TmHU studied by optical tweezers, AFM and molecular dynamics simulations. Journal of Biological Physics, 2011, 37, 117-131.	0.7	7
129	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
130	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
131	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
132	FEMTOSECOND DYNAMICS IN THE ANISOTROPY OF EMISSION IN LH2 UNITS. Nonlinear Optics, Quantum Optics, 2002, 29, 167-172.	0.2	6
133	Treatment of laser-field effects on a molecular wire and its coupling to the leads. Journal of Luminescence, 2008, 128, 1078-1080.	1.5	6
134	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
135	Atomistic Simulation of Molecules Interacting with Biological Nanopores: From Current Understanding to Future Directions. Journal of Physical Chemistry B, 0, , .	1.2	6
136	The mapped Fourier method for scattering problems. Chemical Physics Letters, 1999, 313, 665-669.	1.2	5
137	Different direct integrators for Redfield equations applied to electron transfer dynamics. Journal of Molecular Liquids, 2000, 86, 77-84.	2.3	5
138	Non-Markovian effects in the anisotropy of fluorescence in LH2 units. Journal of Luminescence, 2004, 108, 137-141.	1.5	5
139	The mapping approach in the path integral formalism applied to curve-crossing systems. Chemical Physics, 2004, 296, 149-158.	0.9	5
140	Absorption spectra for a model light-harvesting system using non-Markovian theories. Journal of Luminescence, 2005, 112, 461-464.	1.5	5
141	Density matrix theory for reductive electron transfer in DNA. Journal of Luminescence, 2006, 119-120, 91-95.	1.5	5
142	Relation between Vibrational Dephasing Time and Energy Gap Fluctuations. Journal of Physical Chemistry B, 2017, 121, 6471-6478.	1.2	5
143	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
144	Coherent-state path integral approach to the damped harmonic oscillator. Journal of Physics A, 2004, 37, 3019-3040.	1.6	4

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145	Probing the contributions of hot vibrational states using pump-degenerate four-wave mixing. Chemical Physics Letters, 2009, 470, 39-43.	1.2	4
146	From Atomistic Modeling to Electronic Properties of Light-Harvesting Systems. Semiconductors and Semimetals, 2011, , 83-114.	0.4	4
147	Time-Local Quantum Master Equations and their Applications to Dissipative Dynamics and Molecular Wires. Springer Series in Chemical Physics, 2009, , 339-361.	0.2	4
148	NUMERICAL SIMULATION OF ELECTRON TRANSFER RATES IN BETAINE-30. Nonlinear Optics, Quantum Optics, 2002, 29, 595-601.	0.2	3
149	Sequences of ultrafast non-resonant multiphoton transitions in a three-electronic level molecule. Chemical Physics, 2008, 347, 229-242.	0.9	3
150	Selective Probing of Vibrational Hot States in Bromine Using Time-Resolved Coherent Anti-Stokes Raman Scattering. Journal of Physical Chemistry A, 2012, 116, 11341-11346.	1.1	3
151	Functional Rotation of the Transporter AcrB: The Essentials of Peristaltic Motion and Subsequent Substrate Extrusion. Biophysical Journal, 2010, 98, 685a.	0.2	2
152	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
153	Group three nitride clusters as promising components for nanoelectronics. Materials Today Chemistry, 2022, 23, 100751.	1.7	2
154	Transverse electronic transport through nucleobase-pairs of a DNA wire. Materials Today Chemistry, 2022, 24, 100834.	1.7	2
155	On homogeneous generalized master equations. Journal of Physics A, 2002, 35, 5521-5524.	1.6	1
156	A Monte Carlo method for propagating multi-dimensional wave packets. Physica Status Solidi (B): Basic Research, 2004, 241, 2157-2167.	0.7	1
157	Functional Rotation of the Transporter AcrB: Insights into Drug Extrusion from Simulations. Biophysical Journal, 2010, 98, 628a.	0.2	1
158	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. SSRN Electronic Journal, 0, , .	0.4	1
159	Line defects in quasi-one-dimensional systems: Orthogonality exponents and electron density. Physical Review B, 1993, 48, 4816-4822.	1.1	0
160	FEMTOSECOND DYNAMICS IN THE ANISOTROPY OF EMISSION IN LH2 UNITS. Nonlinear Optics, Quantum Optics, 2002, 29, 151-154.	0.2	0
161	Generalized Heitler-London theory for H 3 : a comparison of the surface integral method with perturbation theory. European Physical Journal D, 2002, 18, 61-68.	0.6	0
162	Simulating Efflux Pumps: The Extrusion Mechanism of Substrates. Biophysical Journal, 2009, 96, 381a-382a.	0.2	0

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163	Simulating Efflux Pumps: Opening of the Exit Duct TolC. Biophysical Journal, 2009, 96, 272a.	0.2	0
164	Ion Transport through OmpF in Molecular Dynamics Simulations and Experiments. Biophysical Journal, 2009, 96, 661a.	0.2	0
165	Theoretische Chemie 2009. Nachrichten Aus Der Chemie, 2010, 58, 331-338.	0.0	0
166	Calculation of optical Properties from Molecular-Dynamics Simulations of Light-Harvesting Systems. Biophysical Journal, 2010, 98, 173a.	0.2	0
167	Probing the Transport of Ionic Liquids in Aqueous Solution through Nanopores. Biophysical Journal, 2012, 102, 205a.	0.2	0
168	Deciphering the Ion Selectivity of the Phosphate Specific Channel OprP from Pseudomonas Aeruginosa: A Free-Energy Molecular Dynamics Simulation Study. Biophysical Journal, 2013, 104, 624a.	0.2	0
169	Environmental Effects in the FMO and PE545 Photosynthetic Complexes. Biophysical Journal, 2014, 106, 181a-182a.	0.2	0
170	Investigating the Structure-Function Relationship of the Phosphate-Selective Channel OprP. Biophysical Journal, 2014, 106, 149a.	0.2	0
171	Environmental Coupling and Population Dynamics in the PE545 Light-Harvesting Complex. Biophysical Journal, 2015, 108, 604a-605a.	0.2	0
172	Understanding the Translocation of Fluoroquinolones through OmpC using the Metadynamics. Biophysical Journal, 2015, 108, 443a.	0.2	0
173	What Keeps TolC Closed? Insights from Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 625a.	0.2	0
174	Dephasing Times in the Phycobiliprotein Antenna Complexes PE545 and PE555. Biophysical Journal, 2017, 112, 442a.	0.2	0
175	Tsx as a Nucleoside Channel. Biophysical Journal, 2017, 112, 450a.	0.2	0
176	Understanding the Structure and Function of the DcaP Channel from Acinetobacter baumannii using MD Simulations. Biophysical Journal, 2018, 114, 491a.	0.2	0