

Toms Kubar

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

43
papers

1,902
citations

21
h-index

43
g-index

47
ext. papers

2,306
ext. citations

5.7
avg, IF

5.01
L-index

#	Paper	IF	Citations
43	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 26366-26375	3.6	0
42	Performance of Mixed Quantum-Classical Approaches on Modeling the Crossover from Hopping to Bandlike Charge Transport in Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2071-2084	6.4	13
41	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. <i>Journal of Chemical Physics</i> , 2020 , 152, 124101	3.9	210
40	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 8660-8667	6.4	14
39	Tetrameric Charge-Zipper Assembly of the TisB Peptide in Membranes-Computer Simulation and Experiment. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 1770-1779	3.4	2
38	What accounts for the different functions in photolyases and cryptochromes: a computational study of proton transfers to FAD. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 11956-11966	3.6	3
37	Orthogonal F-Labeling for Solid-State NMR Spectroscopy Reveals the Conformation and Orientation of Short Peptaibols in Membranes. <i>Chemistry - A European Journal</i> , 2018 , 24, 4328-4335	4.8	10
36	"siRNA traffic lights": arabino-configured 2Tanchors for fluorescent dyes are key for dual color readout in cell imaging. <i>Organic and Biomolecular Chemistry</i> , 2018 , 16, 3726-3731	3.9	4
35	A Molecular Dynamics-Quantum Mechanics Theoretical Study of DNA-Mediated Charge Transport in Hydrated Ionic Liquids. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2733-2742	6.4	6
34	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. <i>Biophysical Journal</i> , 2018 , 114, 2563-2572	2.9	12
33	On the mechanism of spontaneous thiol-disulfide exchange in proteins. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16222-16230	3.6	12
32	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. <i>Journal of Chemical Physics</i> , 2018 , 149, 072328	3.9	8
31	Microsecond Simulation of Electron Transfer in DNA: Bottom-Up Parametrization of an Efficient Electron Transfer Model Based on Atomistic Details. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 529-549	3.4	19
30	Reaction Path Averaging: Characterizing the Structural Response of the DNA Double Helix to Electron Transfer. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 1520-1532	3.4	1
29	Structural Behavior of the Peptaibol Harzianin HK VI in a DMPC Bilayer: Insights from MD Simulations. <i>Biophysical Journal</i> , 2017 , 112, 2602-2614	2.9	5
28	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 286-296	6.4	14
27	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 17985-17997	3.6	8

26	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016 , 116, 5301-37	68.1	210
25	The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 24033-42	3.6	5
24	Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5068-82	6.4	44
23	Parameterization of the DFTB3 method for Br, Ca, Cl, F, I, K, and Na in organic and biological systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 332-42	6.4	164
22	New QM/MM implementation of the DFTB3 method in the gromacs package. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1978-89	3.5	29
21	Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. <i>PLoS ONE</i> , 2015 , 10, e0135399	3.7	4
20	Solvent driving force ensures fast formation of a persistent and well-separated radical pair in plant cryptochrome. <i>Journal of the American Chemical Society</i> , 2015 , 137, 1147-56	16.4	55
19	Fragment orbital based description of charge transfer in peptides including backbone orbitals. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 4261-72	3.4	16
18	Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4242-52	6.4	47
17	Charge transfer in E. coli DNA photolyase: understanding polarization and stabilization effects via QM/MM simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 10769-78	3.4	28
16	Modeling charge transport in DNA using multi-scale methods. <i>Physica Status Solidi (B): Basic Research</i> , 2013 , 250, 2277-2287	1.3	21
15	Parametrization of the SCC-DFTB Method for Halogens. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2939-49	6.4	45
14	Efficient algorithms for the simulation of non-adiabatic electron transfer in complex molecular systems: application to DNA. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 5794-813	3.6	52
13	A hybrid approach to simulation of electron transfer in complex molecular systems. <i>Journal of the Royal Society Interface</i> , 2013 , 10, 20130415	4.1	66
12	Response of the electric conductivity of double-stranded DNA on moderate mechanical stretching stresses. <i>Physical Review B</i> , 2012 , 85,	3.3	19
11	Nonadiabatic QM/MM simulations of fast charge transfer in Escherichia coli DNA photolyase. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9846-63	3.4	69
10	On the structure and stretching of microhydrated DNA. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 11238-47	8.7	11
9	Structural stability versus conformational sampling in biomolecular systems: why is the charge transfer efficiency in G4-DNA better than in double-stranded DNA?. <i>Journal of Chemical Physics</i> , 2010 , 133, 035103	3.9	50

8	Coarse-grained time-dependent density functional simulation of charge transfer in complex systems: application to hole transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 11221-40	3-4	75
7	Structural fluctuations and quantum transport through DNA molecular wires: a combined molecular dynamics and model Hamiltonian approach. <i>New Journal of Physics</i> , 2010 , 12, 023022	2-9	50
6	Charge transport through biomolecular wires in a solvent: bridging molecular dynamics and model Hamiltonian approaches. <i>Physical Review Letters</i> , 2009 , 102, 208102	7-4	77
5	Combined density functional theory and Landauer approach for hole transfer in DNA along classical molecular dynamics trajectories. <i>Journal of Chemical Physics</i> , 2009 , 130, 215104	3-9	73
4	Solvent reorganization energy of hole transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 5653-6	3-4	33
3	Solvent fluctuations drive the hole transfer in DNA: a mixed quantum-classical study. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 13107-17	3-4	68
2	What governs the charge transfer in DNA? The role of DNA conformation and environment. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 8788-98	3-4	109
1	Efficient calculation of charge-transfer matrix elements for hole transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 7937-47	3-4	135