Toms Kubar

List of Publications by Citations

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	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
42	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. *Chemical Reviews*, **2016**, 116, 5301-37	68.1	210
41	Parameterization of the DFTB3 method for Br, Ca, Cl, F, I, K, and Na in organic and biological systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 332-42	6.4	164
40	Efficient calculation of charge-transfer matrix elements for hole transfer in DNA. *Journal of Physical Chemistry B*, **2008**, 112, 7937-47	3.4	135
39	What governs the charge transfer in DNA? The role of DNA conformation and environment. *Journal of Physical Chemistry B*, **2008**, 112, 8788-98	3.4	109
38	Charge transport through biomolecular wires in a solvent: bridging molecular dynamics and model Hamiltonian approaches. *Physical Review Letters*, **2009**, 102, 208102	7.4	77
37	Coarse-grained time-dependent density functional simulation of charge transfer in complex systems: application to hole transfer in DNA. *Journal of Physical Chemistry B*, **2010**, 114, 11221-40	3.4	75
36	Combined density functional theory and Landauer approach for hole transfer in DNA along classical molecular dynamics trajectories. *Journal of Chemical Physics*, **2009**, 130, 215104	3.9	73
35	Nonadiabatic QM/MM simulations of fast charge transfer in Escherichia coli DNA photolyase. *Journal of Physical Chemistry B*, **2011**, 115, 9846-63	3.4	69
34	Solvent fluctuations drive the hole transfer in DNA: a mixed quantum-classical study. *Journal of Physical Chemistry B*, **2009**, 113, 13107-17	3.4	68
33	A hybrid approach to simulation of electron transfer in complex molecular systems. *Journal of the Royal Society Interface*, **2013**, 10, 20130415	4.1	66
32	Solvent driving force ensures fast formation of a persistent and well-separated radical pair in plant cryptochrome. *Journal of the American Chemical Society*, **2015**, 137, 1147-56	16.4	55
31	Efficient algorithms for the simulation of non-adiabatic electron transfer in complex molecular systems: application to DNA. *Physical Chemistry Chemical Physics*, **2013**, 15, 5794-813	3.6	52
30	Structural stability versus conformational sampling in biomolecular systems: why is the charge transfer efficiency in G4-DNA better than in double-stranded DNA?. *Journal of Chemical Physics*, **2010**, 133, 035103	3.9	50
29	Structural fluctuations and quantum transport through DNA molecular wires: a combined molecular dynamics and model Hamiltonian approach. *New Journal of Physics*, **2010**, 12, 023022	2.9	50
28	Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. *Journal of Chemical Theory and Computation*, **2014**, 10, 4242-52	6.4	47
27	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45

26	Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. *Journal of Chemical Theory and Computation*, **2015**, 11, 5068-82	6.4	44
25	Solvent reorganization energy of hole transfer in DNA. *Journal of Physical Chemistry B*, **2009**, 113, 5653-6	3.4	33
24	New QM/MM implementation of the DFTB3 method in the gromacs package. *Journal of Computational Chemistry*, **2015**, 36, 1978-89	3.5	29
23	Charge transfer in E. coli DNA photolyase: understanding polarization and stabilization effects via QM/MM simulations. *Journal of Physical Chemistry B*, **2013**, 117, 10769-78	3.4	28
22	Modeling charge transport in DNA using multi-scale methods. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2277-2287	1.3	21
21	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	3.4	19
20	Response of the electric conductivity of double-stranded DNA on moderate mechanical stretching stresses. *Physical Review B*, **2012**, 85,	3.3	19
19	Fragment orbital based description of charge transfer in peptides including backbone orbitals. *Journal of Physical Chemistry B*, **2014**, 118, 4261-72	3.4	16
18	Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 286-296	6.4	14
17	DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. *Journal of Physical Chemistry Letters*, **2020**, 11, 8660-8667	6.4	14
16	Performance of Mixed Quantum-Classical Approaches on Modeling the Crossover from Hopping to Bandlike Charge Transport in Organic Semiconductors. *Journal of Chemical Theory and Computation* , **2020**, 16, 2071-2084	6.4	13
15	Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. *Biophysical Journal*, **2018**, 114, 2563-2572	2.9	12
14	On the mechanism of spontaneous thiol-disulfide exchange in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 16222-16230	3.6	12
13	On the structure and stretching of microhydrated DNA. *Journal of Physical Chemistry A*, **2011**, 115, 11238-47	2.8	11
12	Orthogonal F-Labeling for Solid-State NMR Spectroscopy Reveals the Conformation and Orientation of Short Peptaibols in Membranes. *Chemistry - A European Journal*, **2018**, 24, 4328-4335	4.8	10
11	Cation solvation with quantum chemical effects modeled by a size-consistent multi-partitioning quantum mechanics/molecular mechanics method. *Physical Chemistry Chemical Physics*, **2017**, 19, 17985-17997	3.6	8
10	Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. *Journal of Chemical Physics*, **2018**, 149, 072328	3.9	8
9	A Molecular Dynamics-Quantum Mechanics Theoretical Study of DNA-Mediated Charge Transport in Hydrated Ionic Liquids. *Journal of Chemical Theory and Computation*, **2018**, 14, 2733-2742	6.4	6

8	Structural Behavior of the Peptaibol Harzianin HK VI in a DMPC Bilayer: Insights from MD Simulations. *Biophysical Journal*, **2017**, 112, 2602-2614	2.9	5
7	The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. *Physical Chemistry Chemical Physics*, **2016**, 18, 24033-42	3.6	5
6	"siRNA traffic lights": arabino-configured 2′-anchors for fluorescent dyes are key for dual color readout in cell imaging. *Organic and Biomolecular Chemistry*, **2018**, 16, 3726-3731	3.9	4
5	Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. *PLoS ONE*, **2015**, 10, e0135399	3.7	4
4	What accounts for the different functions in photolyases and cryptochromes: a computational study of proton transfers to FAD. *Physical Chemistry Chemical Physics*, **2019**, 21, 11956-11966	3.6	3
3	Tetrameric Charge-Zipper Assembly of the TisB Peptide in Membranes-Computer Simulation and Experiment. *Journal of Physical Chemistry B*, **2019**, 123, 1770-1779	3.4	2
2	Reaction Path Averaging: Characterizing the Structural Response of the DNA Double Helix to Electron Transfer. *Journal of Physical Chemistry B*, **2017**, 121, 1520-1532	3.4	1
1	Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. *Physical Chemistry Chemical Physics*, **2021**, 23, 26366-26375	3.6	0