

# Tomáš Kuba

## List of Publications by Year in descending order

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Version: 2024-02-01

46  
papers

2,689  
citations

279798

23  
h-index

214800

47  
g-index

47  
all docs

47  
docs citations

47  
times ranked

2649  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 124101.  | 3.0  | 589       |
| 2  | Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. <i>Chemical Reviews</i> , 2016, 116, 5301-5337.  | 47.7 | 312       |
| 3  | 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, 332-342.  | 5.3  | 227       |
| 4  | Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2008, 112, 7937-7947.   | 2.6  | 150       |
| 5  | What Governs the Charge Transfer in DNA? The Role of DNA Conformation and Environment. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8788-8798.   | 2.6  | 117       |
| 6  | Charge Transport through Biomolecular Wires in a Solvent: Bridging Molecular Dynamics and Model Hamiltonian Approaches. <i>Physical Review Letters</i> , 2009, 102, 208102.   | 7.8  | 80        |
| 7  | 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, 11221-11240.                  | 2.6  | 79        |
| 8  | 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.                                | 3.0  | 78        |
| 9  | Nonadiabatic QM/MM Simulations of Fast Charge Transfer in Escherichia coli DNA Photolyase. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9846-9863.   | 2.6  | 77        |
| 10 | A hybrid approach to simulation of electron transfer in complex molecular systems. <i>Journal of the Royal Society Interface</i> , 2013, 10, 20130415.  | 3.4  | 72        |
| 11 | Solvent Fluctuations Drive the Hole Transfer in DNA: A Mixed Quantum-Classical Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13107-13117.  | 2.6  | 71        |
| 12 | 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, 1147-1156.                               | 13.7 | 70        |
| 13 | 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.                                 | 2.8  | 61        |
| 14 | Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4242-4252.   | 5.3  | 55        |
| 15 | Parametrization of the SCC-DFTB Method for Halogens. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2939-2949.  | 5.3  | 54        |
| 16 | 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  | 53        |
| 17 | Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5068-5082.  | 5.3  | 53        |
| 18 | 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. | 3.0  | 52        |

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|----|---|-----|-----------|
| 19 | New QM/MM implementation of the DFTB3 method in the gromacs package. <i>Journal of Computational Chemistry</i> , 2015, 36, 1978-1989.   | 3.3 | 45        |
| 20 | Solvent Reorganization Energy of Hole Transfer in DNA. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5653-5656.   | 2.6 | 35        |
| 21 | DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8660-8667.   | 4.6 | 34        |
| 22 | 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, 10769-10778.                                   | 2.6 | 33        |
| 23 | Modeling charge transport in DNA using multi-scale methods. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2277-2287.  | 1.5 | 26        |
| 24 | 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.            | 2.6 | 23        |
| 25 | On the mechanism of spontaneous thiol-disulfide exchange in proteins. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 16222-16230.   | 2.8 | 22        |
| 26 | 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. | 5.3 | 21        |
| 27 | Response of the electric conductivity of double-stranded DNA on moderate mechanical stretching stresses. <i>Physical Review B</i> , 2012, 85, .   | 3.2 | 19        |
| 28 | Accurate Free Energies for Complex Condensed-Phase Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1213-1226.                   | 5.3 | 18        |
| 29 | Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. <i>Biophysical Journal</i> , 2018, 114, 2563-2572.  | 0.5 | 17        |
| 30 | Fragment Orbital Based Description of Charge Transfer in Peptides Including Backbone Orbitals. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4261-4272.   | 2.6 | 16        |
| 31 | Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 286-296.  | 5.3 | 16        |
| 32 | Orthogonal <sup>19</sup> 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.              | 3.3 | 14        |
| 33 | Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. <i>Journal of Chemical Physics</i> , 2018, 149, 072328.   | 3.0 | 14        |
| 34 | On the Structure and Stretching of Microhydrated DNA. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11238-11247.  | 2.5 | 13        |
| 35 | 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.          | 2.8 | 10        |
| 36 | Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. <i>PLoS ONE</i> , 2015, 10, e0135399.   | 2.5 | 8         |

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|----|--|-----|-----------|
| 37 | Structural Behavior of the Peptaibol Harzianin HK VI in a DMPC Bilayer: Insights from MD Simulations. <i>Biophysical Journal</i> , 2017, 112, 2602-2614.   | 0.5 | 8         |
| 38 | 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.                        | 5.3 | 7         |
| 39 | The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24033-24042.                                | 2.8 | 6         |
| 40 | 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.  | 2.6 | 6         |
| 41 | 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.                    | 2.8 | 6         |
| 42 | Electrostatic interactions contribute to the control of intramolecular thiol-disulfide isomerization in a protein. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26366-26375.                               | 2.8 | 6         |
| 43 | O to bR transition in bacteriorhodopsin occurs through a proton hole mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .                                | 7.1 | 5         |
| 44 | arabino-configured 2'-anchors for fluorescent dyes are key for dual color readout in cell imaging. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 3726-3731.  | 2.8 | 4         |
| 45 | Unravelling the mechanism of glucose binding in a protein-based fluorescence probe: molecular dynamics simulation with a tailor-made charge model. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2441-2453. | 2.8 | 2         |
| 46 | 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.   | 2.6 | 1         |