# TomÃ¡Å¡ KubaÅ

List of Publications by Year
in descending order

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Version: 2024-02-01

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|---|---|---|---|
| 46 papers | 2,689 citations | 279778 23 h-index | 214788 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. Journal of Chemical Physics, 2020, 152, 124101. | 3.0 | 589 |
| 2 | Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 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. Journal of Chemical Theory and Computation, 2015, 11, 332-342. | 5.3 | 227 |
| 4 | Efficient Calculation of Charge-Transfer Matrix Elements for Hole Transfer in DNA. Journal of Physical Chemistry B, 2008, 112, 7937-7947. | 2.6 | 150 |
| 5 | What Governs the Charge Transfer in DNA? The Role of DNA Conformation and Environment. Journal of Physical Chemistry B, 2008, 112, 8788-8798. | 2.6 | 117 |
| 6 | Charge Transport through Biomolecular Wires in a Solvent: Bridging Molecular Dynamics and Model Hamiltonian Approaches. Physical Review Letters, 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. Journal of Physical Chemistry B, 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. Journal of Chemical Physics, 2009, 130, 215104. | 3.0 | 78 |
| 9 | Nonadiabatic QM/MM Simulations of Fast Charge Transfer in Escherichia coli DNA Photolyase. Journal of Physical Chemistry B, 2011, 115, 9846-9863. | 2.6 | 77 |
| 10 | A hybrid approach to simulation of electron transfer in complex molecular systems. Journal of the Royal Society Interface, 2013, 10, 20130415. | 3.4 | 72 |
| 11 | Solvent Fluctuations Drive the Hole Transfer in DNA: A Mixed Quantumâ^'Classical Study. Journal of Physical Chemistry B, 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. Journal of the American Chemical Society, 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. Physical Chemistry Chemical Physics, 2013, 15, 5794. | 2.8 | 61 |
| 14 | Size-Consistent Multipartitioning QM/MM: A Stable and Efficient Adaptive QM/MM Method. Journal of Chemical Theory and Computation, 2014, 10, 4242-4252. | 5.3 | 55 |
| 15 | Parametrization of the SCC-DFTB Method for Halogens. Journal of Chemical Theory and Computation, 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. New Journal of Physics, 2010, 12, 023022. | 2.9 | 53 |
| 17 | Multi-Scale Approach to Non-Adiabatic Charge Transport in High-Mobility Organic Semiconductors. Journal of Chemical Theory and Computation, 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?. Journal of Chemical Physics, 2010, 133, 035103. | 3.0 | 52 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | New QM/MM implementation of the DFTB3 method in the gromacs package. Journal of Computational Chemistry, 2015, 36, 1978-1989. | 3.3 | 45 |
| 20 | Solvent Reorganization Energy of Hole Transfer in DNA. Journal of Physical Chemistry B, 2009, 113, 5653-5656. | 2.6 | 35 |
| 21 | DFTB/MM Molecular Dynamics Simulations of the FMO Light-Harvesting Complex. Journal of Physical Chemistry Letters, 2020, 11, 8660-8667. | 4.6 | 34 |
| 22 | Charge Transfer in E. coli DNA Photolyase: Understanding Polarization and Stabilization Effects via QM/MM Simulations. Journal of Physical Chemistry B, 2013, 117, 10769-10778. | 2.6 | 33 |
| 23 | Modeling charge transport in DNA using multiâ€scale methods. Physica Status Solidi (B): Basic Research, 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. Journal of Physical Chemistry B, 2017, 121, 529-549. | 2.6 | 23 |
| 25 | On the mechanism of spontaneous thiolâ€“disulfide exchange in proteins. Physical Chemistry Chemical Physics, 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. Journal of Chemical Theory and Computation, 2020, 16, 2071-2084. | 5.3 | 21 |
| 27 | Response of the electric conductivity of double-stranded DNA on moderate mechanical stretching stresses. Physical Review B, 2012, 85, . | 3.2 | 19 |
| 28 | Accurate Free Energies for Complex Condensed-Phase Reactions Using an Artificial Neural Network Corrected DFTB/MM Methodology. Journal of Chemical Theory and Computation, 2022, 18, 1213-1226. | 5.3 | 18 |
| 29 | Molecular Insights into Variable Electron Transfer in Amphibian Cryptochrome. Biophysical Journal, 2018, 114, 2563-2572. | 0.5 | 17 |
| 30 | Fragment Orbital Based Description of Charge Transfer in Peptides Including Backbone Orbitals. Journal of Physical Chemistry B, 2014, 118, 4261-4272. | 2.6 | 16 |
| 31 | Polaron Effects on Charge Transport through Molecular Wires: A Multiscale Approach. Journal of Chemical Theory and Computation, 2017, 13, 286-296. | 5.3 | 16 |
| 32 | Orthogonal <sup>19</sup>Fâ€Labeling for Solidâ€State NMR Spectroscopy Reveals the Conformation and Orientation of Short Peptaibols in Membranes. Chemistry - A European Journal, 2018, 24, 4328-4335. | 3.3 | 14 |
| 33 | Coupled-perturbed DFTB-QM/MM metadynamics: Application to proton-coupled electron transfer. Journal of Chemical Physics, 2018, 149, 072328. | 3.0 | 14 |
| 34 | On the Structure and Stretching of Microhydrated DNA. Journal of Physical Chemistry A, 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. Physical Chemistry Chemical Physics, 2017, 19, 17985-17997. | 2.8 | 10 |
| 36 | Molecular Dynamics Investigation of gluazo, a Photo-Switchable Ligand for the Glutamate Receptor GluK2. PLoS ONE, 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. Biophysical Journal, 2017, 112, 2602-2614. | 0.5 | 8 |
| 38 | 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. | 5.3 | 7 |
| 39 | The effect of the environment on the methyl transfer reaction mechanism between trimethylsulfonium and phenolate. Physical Chemistry Chemical Physics, 2016, 18, 24033-24042. | 2.8 | 6 |
| 40 | Tetrameric Charge-Zipper Assembly of the TisB Peptide in Membranesâ€”Computer Simulation and Experiment. Journal of Physical Chemistry B, 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. Physical Chemistry Chemical Physics, 2019, 21, 11956-11966. | 2.8 | 6 |
| 42 | Electrostatic interactions contribute to the control of intramolecular thiolâ€“disulfide isomerization in a protein. Physical Chemistry Chemical Physics, 2021, 23, 26366-26375. | 2.8 | 6 |
| 43 | O to bR transition in bacteriorhodopsin occurs through a proton hole mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 7.1 | 5 |
| 44 | â€œsiRNA traffic lightsâ€• arabino-configured 2â€²-anchors for fluorescent dyes are key for dual color readout in cell imaging. Organic and Biomolecular Chemistry, 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. Physical Chemistry Chemical Physics, 2022, 24, 2441-2453. | 2.8 | 2 |
| 46 | Reaction Path Averaging: Characterizing the Structural Response of the DNA Double Helix to Electron Transfer. Journal of Physical Chemistry B, 2017, 121, 1520-1532. | 2.6 | 1 |