# Madushanka Manathunga

List of Publications by Year
in descending order



| 15 | 342 | 840585 11 | 996849 15 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 21 | 21 | 21 | 514 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Quantumâ€“classical simulations of rhodopsin reveal excited-state population splitting and its effects on quantum efficiency. Nature Chemistry, 2022, 14, 441-449. | 6.6 | 20 |
| 2 | Computer-aided drug design, quantum-mechanical methods for biological problems. Current Opinion in Structural Biology, 2022, 75, 102417. | 2.6 | 10 |
| 3 | On the Transition from a Biomimetic Molecular Switch to a Rotary Molecular Motor. Journal of Physical Chemistry Letters, 2021, 12, 3875-3884. | 2.1 | 15 |
| 4 | Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK. Journal of Chemical Information and Modeling, 2021, 61, 2109-2115. | 2.5 | 19 |
| 5 | Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2021, 17, 3955-3966. | 2.3 | 15 |
| 6 | Free Energy Computation for an Isomerizing Chromophore in a Molecular Cavity via the Average Solvent Electrostatic Configuration Model: Applications in Rhodopsin and Rhodopsin-Mimicking Systems. Journal of Chemical Theory and Computation, 2021, 17, 5885-5895. | 2.3 | 5 |
| 7 | ReaxFF/AMBERâ€”A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7645-7654. | 2.3 | 19 |
| 8 | Computational and Spectroscopic Characterization of the Photocycle of an Artificial Rhodopsin. Journal of Physical Chemistry Letters, 2020, 11, 4245-4252. | 2.1 | 7 |
| 9 | Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2020, 16, 4315-4326. | 2.3 | 25 |
| 10 | Engineering the vibrational coherence of vision into a synthetic molecular device. Nature Communications, 2018, 9, 313. | 5.8 | 41 |
| 11 | Electronic State Mixing Controls the Photoreactivity of a Rhodopsin with all-trans Chromophore Analogues. Journal of Physical Chemistry Letters, 2018, 9, 6350-6355. | 2.1 | 20 |
| 12 | Impact of Electronic State Mixing on the Photoisomerization Time Scale of the Retinal Chromophore. Journal of Physical Chemistry Letters, 2017, 8, 5222-5227. | 2.1 | 31 |
| 13 | An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems. Journal of Chemical Theory and Computation, 2017, 13, 6391-6404. | 2.3 | 27 |
| 14 | Design, Synthesis, and Dynamics of a Green Fluorescent Protein Fluorophore Mimic with an Ultrafast Switching Function. Journal of the American Chemical Society, 2016, 138, 9807-9825. | 6.6 | 44 |
| 15 | Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. Journal of Chemical Theory and Computation, 2016, 12, 839-850. | 2.3 | 43 |