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	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
2	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. Journal of Chemical Theory and Computation, 2016, 12, 839-850.	2.3	43
3	Engineering the vibrational coherence of vision into a synthetic molecular device. Nature Communications, 2018, 9, 313.	5.8	41
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	Computer-aided drug design, quantum-mechanical methods for biological problems. Current Opinion in Structural Biology, 2022, 75, 102417.	2.6	10
14	Computational and Spectroscopic Characterization of the Photocycle of an Artificial Rhodopsin. Journal of Physical Chemistry Letters, 2020, 11, 4245-4252.	2.1	7
15	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