Federico Melaccio

List of Publications by Year
in descending order

16 papers	724 citations	759055 12 h-index	996849 15 g-index
17 all docs	17 docs citations	17 times ranked	907 citing authors

#	Article	IF	Citations
1	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. Journal of Chemical Theory and Computation, 2014, 10, 3074-3084.	2.3	161
2	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2013, 9, 4495-4506.	2.3	83
3	Using the computer to understand the chemistry of conical intersections. Photochemical and Photobiological Sciences, 2011, 10, 867-886.	1.6	65
4	Toward Automatic Rhodopsin Modeling as a Tool for High-Throughput Computational Photobiology. Journal of Chemical Theory and Computation, 2016, 12, 6020-6034.	2.3	61
5	Quantum chemical modeling of rhodopsin mutants displaying switchable colors. Physical Chemistry Chemical Physics, 2012, 14, 12485.	1.3	60
6	Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1714-1719.	3.3	59
7	Unique QM/MM potential energy surface exploration using microiterations. International Journal of Quantum Chemistry, 2011, 111, 3339-3346.	1.0	55
8	Molecular bases for the selection of the chromophore of animal rhodopsins. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 15297-15302.	3.3	40
9	Computational Photobiology and Beyond. Australian Journal of Chemistry, 2010, 63, 413.	0.5	36
10	Origin of Fluorescence in 11-*cis* Locked Bovine Rhodopsin. Journal of Chemical Theory and Computation, 2012, 8, 2559-2563.	2.3	31
11	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
12	A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore. Angewandte Chemie - International Edition, 2014, 53, 9870-9875.	7.2	21
13	Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment. Journal of Physical Chemistry Letters, 2016, 7, 2563-2567.	2.1	8
14	QM/MM Investigation of the Spectroscopic Properties of the Fluorophore of Bacterial Luciferase. Journal of Chemical Theory and Computation, 2021, 17, 605-613.	2.3	6
15	Computational Photochemistry and Photobiology. , 2012, , 1029-1056.		4
16	Comparative Quantum Chemical Studies of the Ultrafast Isomerization of Microbial, Invertebrate and Vertebrate Rhodopsins. , 2016, , .		0