Stefano Caprasecca

List of Publications by Year
in descending order

27	777	516710 16	580821 25
papers	citations	h-index	g-index

27	27	27	937
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. Journal of Chemical Theory and Computation, 2016, 12, 3654-3661.	5.3	136
2	Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. Journal of Chemical Theory and Computation, 2017, 13, 4025-4033.	5.3	81
3	Toward a Unified Modeling of Environment and Bridge-Mediated Contributions to Electronic Energy Transfer: A Fully Polarizable QM/MM/PCM Approach. Journal of Chemical Theory and Computation, 2012, 8, 4462-4473.	5.3	69
4	An Ab Initio Description of the Excitonic Properties of LH2 and Their Temperature Dependence. Journal of Physical Chemistry B, 2016, 120, 11348-11359.	2.6	64
5	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria. Journal of Physical Chemistry Letters, 2018, 9, 6892-6899.	4.6	55
6	Geometry Optimization in Polarizable QM/MM Models: The Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2014, 10, 1588-1598.	5.3	52
7	Achieving Linear Scaling in Computational Cost for a Fully Polarizable MM/Continuum Embedding. Journal of Chemical Theory and Computation, 2015, 11, 694-704.	5.3	45
8	Combined Experimental and Theoretical Study of Efficient and Ultrafast Energy Transfer in a Molecular Dyad. Journal of Physical Chemistry C, 2014, 118, 23476-23486.	3.1	29
9	Efficient Photoinduced Charge Separation in a BODIPYâ€“C₆₀ Dyad. Journal of Physical Chemistry C, 2016, 120, 16526-16536.	3.1	25
10	Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field. Journal of Physical Chemistry Letters, 2017, 8, 5283-5289.	4.6	25
11	On the description of the environment polarization response to electronic transitions. International Journal of Quantum Chemistry, 2019, 119, e25711.	2.0	25
12	Theoretical Investigation of the Mechanism and Dynamics of Intramolecular Coherent Resonance Energy Transfer in Soft Molecules: A Case Study of Dithia-anthracenophane. Journal of the American Chemical Society, 2010, 132, 16911-16921.	13.7	24
13	Excited-State Gradients in Polarizable QM/MM Models: An Induced Dipole Formulation. Journal of Chemical Theory and Computation, 2017, 13, 3778-3786.	5.3	23
14	Photoprotection and triplet energy transfer in higher plants: the role of electronic and nuclear fluctuations. Physical Chemistry Chemical Physics, 2016, 18, 11288-11296.	2.8	21
15	Plasmon Enhanced Light Harvesting: Multiscale Modeling of the FMO Protein Coupled with Gold Nanoparticles. Journal of Physical Chemistry A, 2015, 119, 5197-5206.	2.5	18
16	Excitation Energy Transfer in Donor-Bridge-Acceptor Systems: A Combined Quantum-Mechanical/Classical Analysis of the Role of the Bridge and the Solvent. Journal of Physical Chemistry A, 2014, 118, 6484-6491.	2.5	17
17	Control of Coherences and Optical Responses of Pigmentâ€“Protein Complexes by Plasmonic Nanoantennae. Journal of Physical Chemistry Letters, 2016, 7, 2189-2196.	4.6	14
18	Theoretical description of protein field effects on electronic excitations of biological chromophores. Journal of Physics Condensed Matter, 2017, 29, 013002.	1.8	10

#	Article	IF	Citations
19	Shaping excitons in light-harvesting proteins through nanoplasmonics. Chemical Science, 2018, 9, 6219-6227.	7.4	9
20	A polarizable QM/MM description of environment effects on NMR shieldings: from solvated molecules to pigmentâ€“protein complexes. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8
21	Quantum mechanical study of the solvent-dependence of electronic energy transfer rates in a Bodipy closely-spaced dyad. Photochemical and Photobiological Sciences, 2011, 10, 1602-1609.	2.9	6
22	Dissecting the Nature of Exciton Interactions in Ethyne-Linked Tetraarylporphyrin Arrays. Journal of Physical Chemistry C, 2013, 117, 12423-12431.	3.1	6
23	Negative solvatochromism of pushâ€“pull biphenyl compounds: a theoretical study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
24	Detection of Stop Sign Violations From Dashcam Data. IEEE Transactions on Intelligent Transportation Systems, 2022, 23, 5411-5420.	8.0	5
25	A quantum chemical investigation of the solvatochromism of a phthalocyanine within a lipid bilayer: Comparison between continuum and atomistic models. Journal of Photochemistry and Photobiology A: Chemistry, 2017, 344, 42-48.	3.9	4
26	Low energy electron collisions with small molecular clusters. Journal of Physics: Conference Series, 2009, 194, 132010.	0.4	0
27	Fault detection in non-reporting Vehicle Tracking Units. , 2019, , .		0