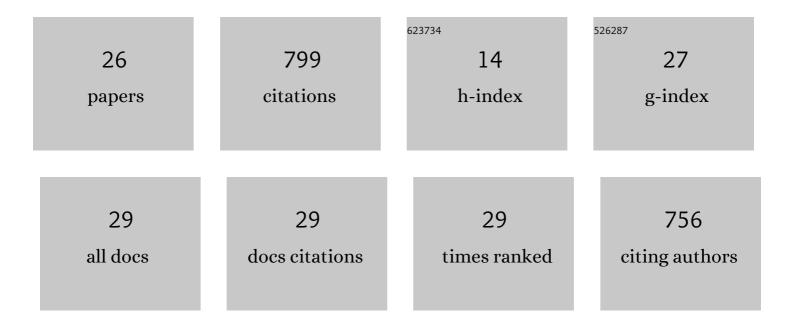
## Marilia T C Martins-Costa

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Photosensitization mechanisms at the air–water interface of aqueous aerosols. Chemical Science, 2022, 13, 2624-2631.	7.4	17
2	Reactivity of Undissociated Molecular Nitric Acid at the Air–Water Interface. Journal of the American Chemical Society, 2021, 143, 453-462.	13.7	14
3	Tight electrostatic regulation of the OH production rate from the photolysis of hydrogen peroxide adsorbed on surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	9
4	Molecular reactions at aqueous interfaces. Nature Reviews Chemistry, 2020, 4, 459-475.	30.2	149
5	The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO <sub>2</sub> in Liquid Water. Journal of the American Chemical Society, 2020, 142, 20937-20941.	13.7	17
6	Photoinduced Oxidation Reactions at the Air–Water Interface. Journal of the American Chemical Society, 2020, 142, 16140-16155.	13.7	38
7	lsoprene Reactivity on Water Surfaces from ab initio QM/MM Molecular Dynamics Simulations. ChemPhysChem, 2020, 21, 2263-2271.	2.1	6
8	Vibrational Sum-Frequency Generation Spectroscopy in the Energy Representation from Dual-Level Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2020, 124, 5675-5683.	2.5	1
9	A New Mechanism of Acid Rain Generation from HOSO at the Air–Water Interface. Journal of the American Chemical Society, 2019, 141, 16564-16568.	13.7	39
10	Theoretical Investigation of the Photoexcited NO <sub>2</sub> +H <sub>2</sub> O reaction at the Air–Water Interface and Its Atmospheric Implications. Chemistry - A European Journal, 2019, 25, 13899-13904.	3.3	14
11	Vibrational Spectroscopy in Solution through Perturbative ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4615-4622.	5.3	9
12	Triplet state promoted reaction of SO <sub>2</sub> with H <sub>2</sub> O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. Physical Chemistry Chemical Physics, 2019, 21, 9779-9784.	2.8	27
13	Photochemistry of SO <sub>2</sub> at the Air–Water Interface: A Source of OH and HOSO Radicals. Journal of the American Chemical Society, 2018, 140, 12341-12344.	13.7	42
14	Cost-Effective Method for Free-Energy Minimization in Complex Systems with Elaborated Ab Initio Potentials. Journal of Chemical Theory and Computation, 2018, 14, 3262-3271.	5.3	7
15	Reaching multiâ€nanosecond timescales in combined QM/MM molecular dynamics simulations through parallel horsetail sampling. Journal of Computational Chemistry, 2017, 38, 659-668.	3.3	19
16	Highly accurate computation of free energies in complex systems through horsetail QM/MM molecular dynamics combined with free-energy perturbation theory. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	9
17	Reactivity of aldehydes at the air–water interface. Insights from molecular dynamics simulations and ab initio calculations. Organic and Biomolecular Chemistry, 2015, 13, 1673-1679.	2.8	23
18	Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. Accounts of Chemical Research, 2015, 48, 575-583.	15.6	90

#	Article	IF	CITATIONS
19	Solvation effects on electronic polarization and reactivity indices at the air–water interface: insights from a theoretical study of cyanophenols. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
20	Advances in QM/MM Molecular Dynamics Simulations of Chemical Processes at Aqueous Interfaces. Challenges and Advances in Computational Chemistry and Physics, 2015, , 303-324.	0.6	5
21	Spectroscopic signatures of ozone at the air–water interface and photochemistry implications. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11618-11623.	7.1	58
22	Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. Journal of the American Chemical Society, 2012, 134, 11821-11827.	13.7	65
23	Reactivity of Atmospherically Relevant Small Radicals at the Air–Water Interface. Angewandte Chemie - International Edition, 2012, 51, 5413-5417.	13.8	69
24	Simulation of amino acid diffusion across water/hydrophobic interfaces. Physical Chemistry Chemical Physics, 2011, 13, 11579.	2.8	14
25	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. Chemistry - A European Journal, 2011, 17, 5076-5085.	3.3	14
26	Free energy calculations using dual-level Born–Oppenheimer molecular dynamics. Journal of Chemical Physics, 2010, 133, 064103.	3.0	22