Marilia T C Martins-Costa

List of Publications by Year
in descending order

26	799	623734	526287
papers	citations	14 h-index	27 g-index

29	29	29	756
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular reactions at aqueous interfaces. Nature Reviews Chemistry, 2020, 4, 459-475.	30.2	149
2	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
3	Reactivity of Atmospherically Relevant Small Radicals at the Airâ€“Water Interface. Angewandte Chemie - International Edition, 2012, 51, 5413-5417.	13.8	69
4	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
5	Spectroscopic signatures of ozone at the airâ€“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
6	Photochemistry of SO₂ at the Airâ€“Water Interface: A Source of OH and HOSO Radicals. Journal of the American Chemical Society, 2018, 140, 12341-12344.	13.7	42
7	A New Mechanism of Acid Rain Generation from HOSO at the Airâ€“Water Interface. Journal of the American Chemical Society, 2019, 141, 16564-16568.	13.7	39
8	Photoinduced Oxidation Reactions at the Airâ€“Water Interface. Journal of the American Chemical Society, 2020, 142, 16140-16155.	13.7	38
9	Triplet state promoted reaction of SO₂ with H₂O 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
10	Reactivity of aldehydes at the airâ€“water interface. Insights from molecular dynamics simulations and ab initio calculations. Organic and Biomolecular Chemistry, 2015, 13, 1673-1679.	2.8	23
11	Free energy calculations using dual-level Bornâ€“Oppenheimer molecular dynamics. Journal of Chemical Physics, 2010, 133, 064103.	3.0	22
12	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
13	The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO₂ in Liquid Water. Journal of the American Chemical Society, 2020, 142, 20937-20941.	13.7	17
14	Photosensitization mechanisms at the airâ€“water interface of aqueous aerosols. Chemical Science, 2022, 13, 2624-2631.	7.4	17
15	Simulation of amino acid diffusion across water/hydrophobic interfaces. Physical Chemistry Chemical Physics, 2011, 13, 11579.	2.8	14
16	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. Chemistry - A European Journal, 2011, 17, 5076-5085.	3.3	14
17	Theoretical Investigation of the Photoexcited NO₂+H₂O reaction at the Airâ€“Water Interface and Its Atmospheric Implications. Chemistry - A European Journal, 2019, 25, 13899-13904.	3.3	14
18	Reactivity of Undissociated Molecular Nitric Acid at the Airâ€“Water Interface. Journal of the American Chemical Society, 2021, 143, 453-462.	13.7	14

#	Article	IF	Citations
19	Solvation effects on electronic polarization and reactivity indices at the airâ€“water interface: insights from a theoretical study of cyanophenols. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
20	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
21	Vibrational Spectroscopy in Solution through Perturbative ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 4615-4622.	5.3	9
22	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
23	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
24	Isoprene Reactivity on Water Surfaces from abâ€…initio QM/MM Molecular Dynamics Simulations. ChemPhysChem, 2020, 21, 2263-2271.	2.1	6
25	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
26	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