

Marilia T C Martins-Costa

List of Publications by Year in descending order

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26
papers

799
citations

623734

14
h-index

526287

27
g-index

29
all docs

29
docs citations

29
times ranked

756
citing authors

#	ARTICLE	IF	CITATIONS
1	Photosensitization mechanisms at the air–water interface of aqueous aerosols. <i>Chemical Science</i> , 2022, 13, 2624-2631.	7.4	17
2	Reactivity of Undissociated Molecular Nitric Acid at the Air–Water Interface. <i>Journal of the American Chemical Society</i> , 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. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	9
4	Molecular reactions at aqueous interfaces. <i>Nature Reviews Chemistry</i> , 2020, 4, 459-475.	30.2	149
5	The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO ₂ in Liquid Water. <i>Journal of the American Chemical Society</i> , 2020, 142, 20937-20941.	13.7	17
6	Photoinduced Oxidation Reactions at the Air–Water Interface. <i>Journal of the American Chemical Society</i> , 2020, 142, 16140-16155.	13.7	38
7	Isoprene Reactivity on Water Surfaces from ab Initio QM/MM Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2020, 21, 2263-2271.	2.1	6
8	Vibrational Sum-Frequency Generation Spectroscopy in the Energy Representation from Dual-Level Molecular Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5675-5683.	2.5	1
9	A New Mechanism of Acid Rain Generation from HOSO at the Air–Water Interface. <i>Journal of the American Chemical Society</i> , 2019, 141, 16564-16568.	13.7	39
10	Theoretical Investigation of the Photoexcited NO ₂ +H ₂ O reaction at the Air–Water Interface and Its Atmospheric Implications. <i>Chemistry - A European Journal</i> , 2019, 25, 13899-13904.	3.3	14
11	Vibrational Spectroscopy in Solution through Perturbative ab Initio Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4615-4622.	5.3	9
12	Triplet state promoted reaction of SO ₂ with H ₂ O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9779-9784.	2.8	27
13	Photochemistry of SO ₂ at the Air–Water Interface: A Source of OH and HOSO Radicals. <i>Journal of the American Chemical Society</i> , 2018, 140, 12341-12344.	13.7	42
14	Cost-Effective Method for Free-Energy Minimization in Complex Systems with Elaborated Ab Initio Potentials. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3262-3271.	5.3	7
15	Reaching multi-nanosecond timescales in combined QM/MM molecular dynamics simulations through parallel horsetail sampling. <i>Journal of Computational Chemistry</i> , 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. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	1.4	9
17	Reactivity of aldehydes at the air–water interface. Insights from molecular dynamics simulations and ab initio calculations. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 1673-1679.	2.8	23
18	Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. <i>Accounts of Chemical Research</i> , 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. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	13
20	Advances in QM/MM Molecular Dynamics Simulations of Chemical Processes at Aqueous Interfaces. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 303-324.	0.6	5
21	Spectroscopic signatures of ozone at the air–water interface and photochemistry implications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 11618-11623.	7.1	58
22	Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. <i>Journal of the American Chemical Society</i> , 2012, 134, 11821-11827.	13.7	65
23	Reactivity of Atmospherically Relevant Small Radicals at the Air–Water Interface. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5413-5417.	13.8	69
24	Simulation of amino acid diffusion across water/hydrophobic interfaces. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11579.	2.8	14
25	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. <i>Chemistry - A European Journal</i> , 2011, 17, 5076-5085.	3.3	14
26	Free energy calculations using dual-level Born–Oppenheimer molecular dynamics. <i>Journal of Chemical Physics</i> , 2010, 133, 064103.	3.0	22