Marcos Felipe Calegari Andrade

List of Publications by Year
in descending order

8	735	1163117	1588992
papers	citations	8	8
		h-index	g-index

8	8	8	892
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab initio theory and modeling of water. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10846-10851.	7.1	340
2	Free energy of proton transfer at the water–TiO$_2$ interface from *ab initio* deep potential molecular dynamics. Chemical Science, 2020, 11, 2335-2341.	7.4	134
3	Raman spectrum and polarizability of liquid water from deep neural networks. Physical Chemistry Chemical Physics, 2020, 22, 10592-10602.	2.8	80
4	Structure, Polarization, and Sum Frequency Generation Spectrum of Interfacial Water on Anatase TiO$_2$. Journal of Physical Chemistry Letters, 2018, 9, 6716-6721.	4.6	70
5	When do short-range atomistic machine-learning models fall short?. Journal of Chemical Physics, 2021, 154, 034111.	3.0	61
6	Effects of applied voltage on water at a gold electrode interface from *ab initio* molecular dynamics. Chemical Science, 2021, 12, 5865-5873.	7.4	29
7	Hydrogen Dynamics in Supercritical Water Probed by Neutron Scattering and Computer Simulations. Journal of Physical Chemistry Letters, 2020, 11, 9461-9467.	4.6	11
8	Structure of disordered TiO_2 phases from *ab initio* based deep neural network simulations. Physical Review Materials, 2020, 4, .	2.4	10