

Marcos Felipe Calegari Andrade

List of Publications by Year in descending order

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Version: 2024-02-01

8
papers

735
citations

1163117
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1588992
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all docs

8
docs citations

8
times ranked

892
citing authors

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