Fabrizio Creazzo

List of Publications by Year
in descending order

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11 papers	199 citations	1307594 7 h-index	1281871 11 g-index
11 all docs	11 docs citations	11 times ranked	237 citing authors

#	Article	IF	Citations
1	Closer Look at Inverse Electron Demand Dielsâ€“Alder and Nucleophilic Addition ReactionsÂon s-Tetrazines Using Enhanced Sampling Methods. Topics in Catalysis, 2022, 65, 1-17.	2.8	2
2	Machine Learning-Assisted Discovery of Hidden States in Expanded Free Energy Space. Journal of Physical Chemistry Letters, 2022, 13, 1797-1805.	4.6	7
3	Effects of surface wettability on (001)-WO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e753" altimg="si81.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math> and (100)-WSe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e761" altimg="si84.svg"><mml:msub><mml:mrow	6.1	1
4	Waterâ€Assisted Chemical Route Towards the Oxygen Evolution Reaction at the Hydrated (110) Ruthenium Oxide Surface: Heterogeneous Catalysis via DFTâ€MD and Metadynamics Simulations. Chemistry - A European Journal, 2021, 27, 17024-17037.	3.3	4
5	Explicit solvent effects on (1 1 0) ruthenium oxide surface wettability: Structural, electronic and mechanical properties of rutile RuO2 by means of spin-polarized DFT-MD. Applied Surface Science, 2021, 570, 150993.	6.1	13
6	Ions Tune Interfacial Water Structure and Modulate Hydrophobic Interactions at Silica Surfaces. Journal of the American Chemical Society, 2020, 142, 6991-7000.	13.7	53
7	Enhanced conductivity of water at the electrified airâ€“water interface: a DFT-MD characterization. Physical Chemistry Chemical Physics, 2020, 22, 10438-10446.	2.8	12
8	DFT-MD of the (110)-Co3O4 cobalt oxide semiconductor in contact with liquid water, preliminary chemical and physical insights into the electrochemical environment. Journal of Chemical Physics, 2019, 150, 041721.	3.0	23
9	Ionic diffusion and proton transfer of MgCl₂ and CaCl₂ aqueous solutions: an ab initio study under electric field. Molecular Simulation, 2019, 45, 373-380.	2.0	8
10	Ionic diffusion and proton transfer in aqueous solutions of alkali metal salts. Physical Chemistry Chemical Physics, 2017, 19, 20420-20429.	2.8	40
11	Ab initio molecular dynamics study of an aqueous NaCl solution under an electric field. Physical Chemistry Chemical Physics, 2016, 18, 23164-23173.	2.8	36