A Roldan

List of Publications by Year
in descending order

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11 papers	558 citations	840776 11 h-index	1281871 11 g-index
11 all docs	11 docs citations	11 times ranked	778 citing authors

#	Article	IF	Citations
1	Density Functional Theory Study of Ni Clusters Supported on the ZrO₂(111) Surface. Fuel Cells, 2017, 17, 125-131.	2.4	16
2	DFT-D2 simulations of water adsorption and dissociation on the low-index surfaces of mackinawite (FeS). Journal of Chemical Physics, 2016, 144, 174704.	3.0	33
3	Catalytic water dissociation by greigite Fe ₃ S ₄ surfaces: density functional theory study. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2016, 472, 20160080.	2.1	17
4	Surface and shape modification of mackinawite (FeS) nanocrystals by cysteine adsorption: a first-principles DFT-D2 study. Physical Chemistry Chemical Physics, 2016, 18, 32007-32020.	2.8	35
5	DFT-D2 Study of the Adsorption and Dissociation of Water on Clean and Oxygen-Covered {001} and {011} Surfaces of Mackinawite (FeS). Journal of Physical Chemistry C, 2016, 120, 21441-21450.	3.1	34
6	Methanol formation from CO₂catalyzed by Fe₃S₄{111}: formate versus hydrocarboxyl pathways. Faraday Discussions, 2016, 188, 161-180.	3.2	29
7	Bio-inspired CO₂conversion by iron sulfide catalysts under sustainable conditions. Chemical Communications, 2015, 51, 7501-7504.	4.1	188
8	Activation and dissociation of CO2 on the (001), (011), and (111) surfaces of mackinawite (FeS): A dispersion-corrected DFT study. Journal of Chemical Physics, 2015, 143, 094703.	3.0	46
9	The surface chemistry of NO_x on mackinawite (FeS) surfaces: a DFT-D2 study. Physical Chemistry Chemical Physics, 2014, 16, 15444-15456.	2.8	40
10	A comparative DFT study of the mechanical and electronic properties of greigite Fe3S4 and magnetite Fe3O4. Journal of Chemical Physics, 2013, 138, 204712.	3.0	75
11	Adsorption of methylamine on mackinawite (FES) surfaces: A density functional theory study. Journal of Chemical Physics, 2013, 139, 124708.	3.0	45