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	Bio-inspired CO₂conversion by iron sulfide catalysts under sustainable conditions. Chemical Communications, 2015, 51, 7501-7504.	4.1	188
2	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
3	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
4	Adsorption of methylamine on mackinawite (FES) surfaces: A density functional theory study. Journal of Chemical Physics, 2013, 139, 124708.	3.0	45
5	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
6	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
7	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
8	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
9	Methanol formation from CO₂catalyzed by Fe₃S₄{111}: formate versus hydrocarboxyl pathways. Faraday Discussions, 2016, 188, 161-180.	3.2	29
10	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
11	Density Functional Theory Study of Ni Clusters Supported on the ZrO₂(111) Surface. Fuel Cells, 2017, 17, 125-131.	2.4	16