Giuliano Carchini

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	On the properties of binary rutile MO2 compounds, M = Ir, Ru, Sn, and Ti: A DFT study. Journal of Chemical Physics, 2013, 138, 194706.	3.0	50
2	State-of-the-art and challenges in theoretical simulations of heterogeneous catalysis at the microscopic level. Catalysis Science and Technology, 2012, 2, 2405.	4.1	38
3	A theoretical study of gas adsorption on calcite for CO2 enhanced natural gas recovery. Applied Surface Science, 2020, 504, 144575.	6.1	28
4	Effect of rock mineralogy on Hot-CO2 injection for enhanced gas recovery. Journal of Natural Gas Science and Engineering, 2019, 72, 103030.	4.4	19
5	Effect of surface morphology on methane interaction with calcite: a DFT study. RSC Advances, 2020, 10, 16669-16674.	3.6	17
6	How Theoretical Simulations Can Address the Structure and Activity of Nanoparticles. Topics in Catalysis, 2013, 56, 1262-1272.	2.8	16
7	Adsorption of small mono- and poly-alcohols on rutile TiO2: a density functional theory study. Physical Chemistry Chemical Physics, 2014, 16, 14750.	2.8	13
8	A theoretical study of gas adsorption on α-quartz (0Â0Â1) for CO2 enhanced natural gas recovery. Applied Surface Science, 2020, 525, 146472.	6.1	10
9	Influence of natural gas composition on adsorption in calcite Nanopores: A DFT study. Applied Surface Science, 2021, 568, 150940.	6.1	8
10	Ab Initio Molecular Dynamics Investigation of CH ₄ /CO ₂ Adsorption on Calcite: Improving the Enhanced Gas Recovery Process. ACS Omega, 2020, 5, 30226-30236.	3.5	6
11	Effect of strain on gas adsorption in tight gas carbonates: A DFT study. Computational Materials Science, 2021, 188, 110186.	3.0	5
12	Ab-Initio Molecular Dynamics investigation of gas adsorption on α-quartz (001) for CO2 enhanced natural gas recovery. Journal of Petroleum Science and Engineering, 2021, 205, 108963.	4.2	2
13	Molecular dynamics of <scp>CH₄</scp> / <scp>CO₂</scp> on calcite for enhancing gas recovery. Canadian Journal of Chemical Engineering, 2022, 100, 3184-3195.	1.7	2