## **Giuliano Carchini**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Molecular dynamics of <scp>CH<sub>4</sub></scp> CO <sub>2</sub> on calcite for enhancing gas recovery. Canadian Journal of Chemical Engineering, 2022, 100, 3184-3195.	1.7	2
2	Effect of strain on gas adsorption in tight gas carbonates: A DFT study. Computational Materials Science, 2021, 188, 110186.	3.0	5
3	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
4	Influence of natural gas composition on adsorption in calcite Nanopores: A DFT study. Applied Surface Science, 2021, 568, 150940.	6.1	8
5	A theoretical study of gas adsorption on calcite for CO2 enhanced natural gas recovery. Applied Surface Science, 2020, 504, 144575.	6.1	28
6	Ab Initio Molecular Dynamics Investigation of CH <sub>4</sub> /CO <sub>2</sub> Adsorption on Calcite: Improving the Enhanced Gas Recovery Process. ACS Omega, 2020, 5, 30226-30236.	3.5	6
7	Effect of surface morphology on methane interaction with calcite: a DFT study. RSC Advances, 2020, 10, 16669-16674.	3.6	17
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	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
10	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
11	How Theoretical Simulations Can Address the Structure and Activity of Nanoparticles. Topics in Catalysis, 2013, 56, 1262-1272.	2.8	16
12	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
13	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