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Computational Study of the Separation of Natural Gas Components in Anion-Pillared Metal-Organic Frameworks (APMOFs)

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To meet the proposals of the United Nations Framework Convention on Climate Change (UNFCCC) held in 2015, natural gas has been studied as a transitional energy matrix due to its low emission of greenhouse gases[1]. However, it contains undesirable compounds such as N_2, NO_X, H_2S, and some light hydrocarbons ($C_{2\text{-}4}H_S$). The search for materials capable of separating these gases has become a field of significant scientific development, with metal-organic frameworks (MOFs) being strong candidates for this purpose[2,3]. Therefore, this study aims to investigate how the MOFs CrOFOUR-1-Ni and MoOFOUR-1-Ni function in the separation of gases present in natural gas at a theoretical level. For this purpose, the Density Functional Theory (DFT) formalism was used for structural optimization, presenting an average error of less than 0,01% in lattice parameters. The simulation of the CH_4 adsorption isotherm was carried out in RASPA (Figure 1), showing good agreement with experimental results. The adsorption of other light hydrocarbons is going to be presented.

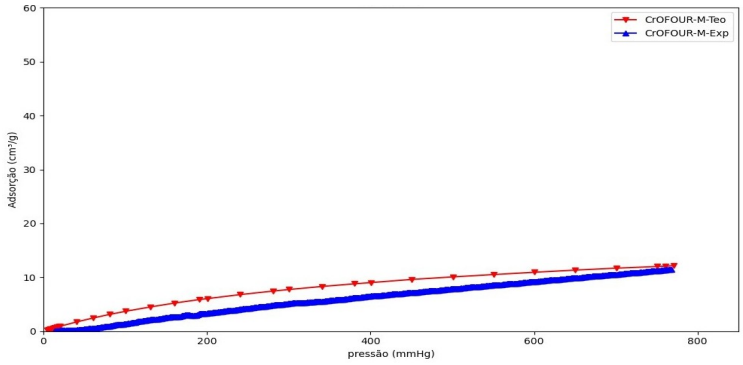

Figure 1: Methane adsorption in CrOFOUR-1-Ni

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