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Theorical Studies of CO_2 Capture in Structured and Humid Nanopores

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Abstract: Metal-Organic Frameworks (MOFs) constitute a crystalline material class that has been heavily studied since the last decade and they present structured nanopores [1-5]. MOFs are built coordinating metallic ions with organic multifunctional binders [6]. The combination of organic functional groups with specific inorganic unities allow infinite different arranges to be possible, while presenting unique properties and easy modulation [7]. The ability to identify and capture a variety of gas molecule based on the interaction affinity between a MOF and the gas is highly desirable. That would reduce the financial cost and the time needed to capture undesirable molecules in the atmosphere, like CO_2, for example. Computational simulations might offer a microscopic perspective about the interactions between the molecules, which is inaccessible with experimental measures.

This work is organized in two steps. At first, simulations considering infinitely long MOFs with CO_2 and Metane gases are compared to previously done simulations. The second part consist of finite MOFs, of different sizes, along with atmosphere gases simulations to identify the effect of humidity in the system. The MOF considered in this work simulations is zinc-methylimidazolate framework-8 (ZIF-8).

The goal of this work is to develop and validate computational methodologies with low processing cost that can identify MOFs with potential to capture CO_2. Then, the expected results are: (i) develop and validate different force fields for the Monte Carlo computational simulations, using the software DICE [8], to describe the process of absorption and liberation of molecules from the atmosphere in the MOFs; (ii) identify the effects of finite sized MOFs for gas capture; (iii) identify how humidity affect the MOFs and the consequences on gas capture.

Key-words: MOF, Atmosphere, Monte Carlo, Computational Simulation, Carbon Dioxide

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