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METAL-ORGANIC FRAMEWROKS: PHYSICAL CHARACTERISTICS, TRANSPORT PHENOMENA AND THE BREATHING EFFECT

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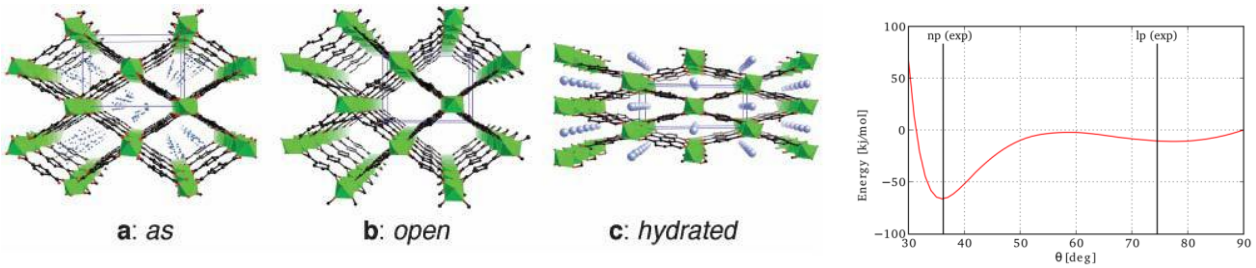
Metal Organic Frameworks (MOFs) can be considered as the most recent development in the field of ordered porous materials, and in a way they close the circle that was initiated about 50 years ago. Needing larger pores than the typical 8 – 12 rings that can be found in zeolites with typical dimensions of 0.2 -2 nm, scientists opened a new area of research and developed many templated supramolecular assemblies, that had larger pores but were not atomically ordered. Metal Organic Frameworks now close the circle; they are crystalline atomically ordered porous materials, with an almost unlimited choice of building bricks, allowing a very precise control over morphology, pore size and functionalities in the walls (as shown in Figure 1). These exceptional properties have brought these hybrid materials to the attention of many research groups in both academia and industry, with over 1000 publications on an annual basis and many of them appeared in the highest impact journals such as Nature, Science,… due to the exceptional promises for energy storage, catalysis, energy-related gas separations.

An intriguing property of many MOFs is that of framework flexibility. They are prone to drastic volume changes due to strong host-guest interactions while keeping the same topology. (See figure.) These volume changes are heavily dependent on the molecules trapped in the pores of the material. This property can lead to a 'gate-opening' phenomenon where a guest molecule is able to pass through a pore that would apparently seem too narrow when measured from the static crystal structure. Another manifestation of the framework flexibility is that of 'pore' breathing, where the whole structure can expand to admit guest molecules, with an analogous shrinking of the overall pore structure under desorption conditions.



Goal Within this proposal, we will investigate theoretically the framework flexibility. The breathing needs to be studied both for the unloaded and loaded MOFs with various guest molecules, as it has been clearly shown that the effect is very sensitive to the type of molecules present in the pores. The major outcome of this study is the physical interpretation of why the structure breaths and under

influence of which host-guest interactions. The breathing will obviously have a major impact on the diffusion and transport phenomena of the mobile phase within the pores of the materials.

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