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Adsorption of nitrogenous species: a theoretical study on the MOFs SIFSIX-3-Cu and SISFIX-2-Cu-i

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Ammonia (NH_3) is a highly versatile and important chemical compound. Its derivatives find applications ranging from use as a fertilizer in agriculture to its presence in cleaning products and pharmaceuticals. However, its production and synthesis often involve other nitrogenous compounds that are either pollutants or do not hold the same market value. Therefore, it is necessary to develop and improve techniques for the selective separation, capture, and storage of ammonia in relation to mixtures containing other nitrogenous species. This ensures the maximization of the benefits associated with the use of NH3 derivatives in various industrial areas.

In this context, Metal-Organic Frameworks (MOFs) emerged as promising materials to play this role. Defined as coordination polymers with potential voids, these structures have cavities that interacted with molecules to confine them within the formed pores. In this study, the adsorption capacities of the compounds NH_3, NO , NO_2 and N_2 by the MOFs SIFSIX-3-Cu and SIFSIX-2-Cu-i were investigated. For this purpose, a theoretical methodology based on classical calculations was adopted, which included Monte Carlo and Molecular Dynamics simulations and structural studies, using the Quantum Espresso and RASPA software.

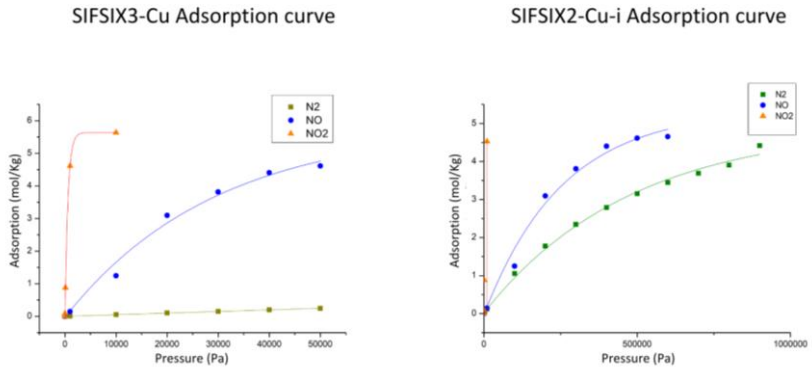

Figure 1 - Adsorption curve for the MOFs sifsix3 and sifsix31, respectively

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References

[1] Guimarães, W. G., Lima, G. F., J. Mol. Model. **26**,1-11 (2020).
[2] Grigoletto, Sabrina, et al. Physical Chemistry Chemical Physics **25**.40 (2023): 27532-27541.