EFFECT OF COEXISTING IMPURITIES ON THE ADSORPTION OF CO_2 IN POROUS MATERIALS[1]

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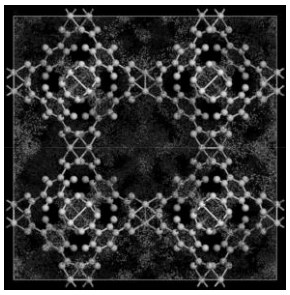
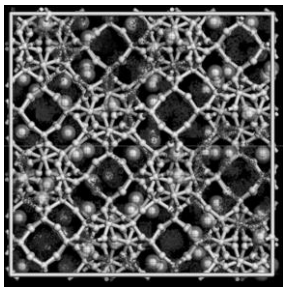
CO_2 adsorption and separation processes over MOFs and zeolites have been intensely studied by means of experimental techniques and computational simulations in recent years, however, and in spite of the great importance from their practical implementation, the investigation of the effect of coexisting components or impurities in flue gases (i.e., water, SO_2 and others) is less explored[2]. Those impurities may significantly influence the stability and the performance of the materials. However, the necessary understanding about the influence of the main components in flue gas on the CO_2 adsorption behaviour in these materials still needs further investigation, which is one of the main objectives of the present work.

CuBTC



Faujasite 13X



Thus, a comparative computational investigation for CO_2 separation of multicomponent mixtures with a composition typical of flue gas is performed using two representative materials, i.e. MOF CuBTC (a.k.a. HKUST-1) and zeolite 13X. Grand Canonical Monte Carlo simulations (GCMC) were used to obtain adsorption isotherms for the pure components CO_2, N_2, H_2O, O_2 and SO_2, as well as for their binary and multicomponent mixtures with CO_2. The influence of the main flue gas components on CO_2 capacity of the material at different conditions was obtained and discussed, as well as selectivity, isosteric heats, adsorption sites location, and the changes that impurities such as water and SO_2 produce in these properties. The main focus on this work was on quantifying the effect of water and impurities on the adsorption behaviour, at the molecular and macroscopic level, and, hence, on the influence at real operating conditions. As a further step, the simulation results were used to analyse the separation of CO_2 from the gas stream at PSA, VSA and TSA processes for the regeneration of both adsorbents.

References
[1] D. Bahamon, A. Díaz-Márquez, P. Gamallo, L. F. Vega, *(submitted)*
[2] J. Yu, Y. Ma, P. B. Balbuena, *Langmuir.* **2012**, *28*, 8064