

EFFECT OF Na^+ ADDITION IN THE ADSORPTION OF O_2 , N_2 AND CO_2 ON FAUJASITE FRAMEWORKS: A DFT STUDY

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Zeolites are widely used materials for many industrial processes. Depending on the zeolite, they can be used as water adsorbents, reversible cation exchangers, hydrocarbon separators, gas separators or catalysts. The main factor that controls the activity of the zeolite is the so-called Si/Al ratio that represents the quantity of AlO_2^- units per cell. The presence of aluminum atoms originates negative charges that need alkali or alkali earth cations to get balanced. Faujasite [1] is a zeolite that belongs to the FAU framework with a Si/Al ratio of 2.4 and widely used in processes that involve capture of CO_2 .

In order to evaluate the optimum faujasite Si/Al ratio observed in CO_2 capture processes a DFT study is proposed. Thus, N_2 , O_2 and CO_2 interactions with Faujasite frameworks at different Si/Al ratios were obtained (i.e., from fully silicated faujasite to 3.36 Si/Al ratio), showing that the presence of aluminum/cation pairs strongly affects the diffusion barriers of adsorbents found in the porous material as well as their binding energies [2]. The values obtained here are important in order to get new force fields that describe correctly the CO_2 capture in flue gas mixtures, the common outgoing gases in many industries.

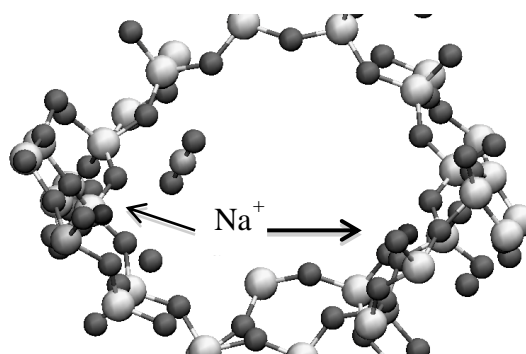


Fig.1. Faujasite detail with CO_2 molecule adsorbed in a site II Na^+

- 1) Ch. Baerlocher, L.B. McCusker, D.H. Olson. *Atlas of Zeolite Framework Types* (6th Ed). 2007, Elsevier
- 2) H.V. Thang, L. Grajciar, et. al. *Catalysis Today*, 2014, 227, 50-56