[1] S. G. Johnson, J. D. Joannopoulos, Photonic crystrals: The road from theory to practice. Springer, USA, 2001.

[2] Y. A. Vlasov, *et al. Phys. Rev. E* **61**, 5784–5793 (2000).

[3] J.-M. Meijer, *et al. Langmuir* **28**, 7631−7638 (2012).

[4] H. Miguez, *et al. Adv. Mater.* **10**, 480-483 (1998).

[5] G. Herzog, *et al. Langmuir* **28**, 8230−8237 (2012).

[6] A.V. Zozulya, *et al. J. Appl. Cryst.* **46**, 903−907 (2013).

[7] E.A. Sulyanova, *et al. Langmuir*, published online (2015).

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MS17-P15 How do zeolite capture CO_2? in-situ synchrotron XRPD investigation of gas asdorption in FAU systems

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The separation of CO_2 from other light gases has been largely practiced in the past. In particular, much of the work concerned the separation of CO_2 for the purification of natural gas[1]. More recently, great emphasis has been given to CO_2 separation from the flue gases associated with combustion processes [2,3]. This interest is directly linked to the importance of CO_2 as a key anthropogenic greenhouse gas, strictly linked to global climate changes [4]. In this work we describe the positions and the interactions of the CO_2 molecules adsorbed in zeolite cavities, on the basis of *in situ* synchrotron X-Ray Powder Diffraction (XRPD) experiments performed at the MCX beamline at Elettra Sincrotrone Trieste source. Three different zeolite samples were investigated: NaX, NaY and CaLSX. They share the same FAU framework type, but have different Si/Al ratios and cation contents. After a HT treatment, carried out to remove the water molecules hosted in the channels, the samples were saturated with CO_2 at 1 bar for 30 minutes and XRPD patterns were collected on an image plate at a fixed wavelength. In order to study the CO_2 desorption behavior, a series of patterns was collected upon heating from room T to 600°C. The experiments show that CO_2 was successfully adsorbed in the zeolite channels of all the samples. Forty-eight and forty CO_2 molecules were localized in Na-Y and Ca-LSX supercage, respectively. In the sodic sample the molecules-cation interactions are water mediated, while in the Ca phase the CO_2 molecules directly interact with the cation sited in the supercage. In the Na-X sample five Na-coordinated CO_2 molecules were localized in the sodalitic cage, while carbonate-like species were found near the supercage. Due to the low number of CO_2 molecules found by this structure refinement, we can not exclude that further molecules are present in the cages with a disordered distribution. Upon heating up to 600°C, NaX and NaY underwent a complete release of all the previously adsorbed CO_2 molecules. On the contrary, Ca-LSX retained 25 CO_2 molecules, suggesting a stronger bonding interaction with Ca cations in the channels.

References: [1] S. Sridhar, B. Smitha, T. M. Aminabhavi, Sep. Purif. Rev. 2007, 36, 113. [2] D. Aaron, C. Tsouris, Sep. Purif. Rev. 2005, 40, 321. [3] H. Balat, C. Oz, Energy Explor. Exploit. 2007, 25, 357. [4] H. Yang, et al. , J.Environ. Sci. (Beijing, China) 2008, 20, 14.

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