CO_2 and N_2 behavior within the LTA zeolite.

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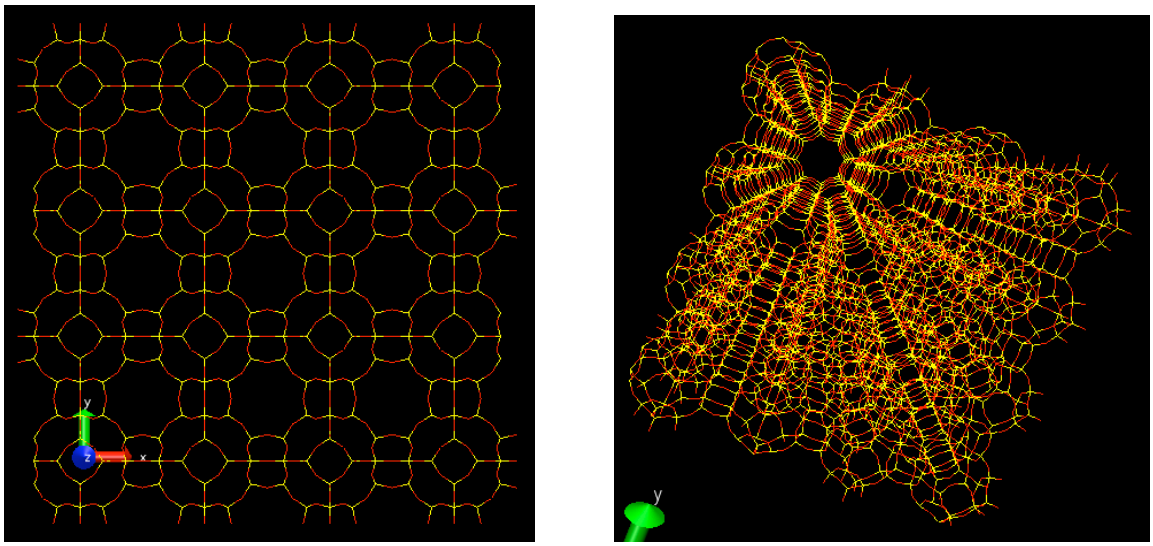
The behavior of molecules inside the nanometer-scale pores of zeolites controls the performance of zeolites in many applications including chemical separations and catalysis.

Previous molecular dynamics studies investigated the influence of pore geometry on the diffusion behavior of CO_2, N_2 and CO_2/N_2 mixtures in three zeolites with identical chemical composition (SiO_2) but different structures. These studies show that the behavior is quite different within the one material with cages (ITQ-3) and the two materials with channels (ITQ-7 and silicalite) that were examined.[1,2]

ZK4, structure type LTA is another zeolite that contains cages (alpha) and is an all silica zeolite (see picture below). It is therefore an ideal candidate to try to elucidate if the behavior exhibited by CO_2 within ITQ-3 can be generalized to other zeolites with cages. Here we describe our efforts to use Molecular Dynamics and Grand Canonical Monte Carlo techniques to reveal the diffusion behavior of CO_2 and N_2 and their mixtures within ZK4. Results include a comparison of diffusion among the four zeolites mentioned as well as a probability map showing the likely sites of CO_2 and N_2 adsorption in ZK4.



LTA crystalline structure showing four unit cells. Red represents oxygen, yellow represents silicon. The image on the left shows the 3D structure in the X-Y plane. The image on the right shows a channel of diffusion created by the connection of the alpha cages.

(1) Goj, A.; Sholl, D. S.; Akten, E. D.; Kohen, D. *Journal of Physical Chemistry B* **2002**, *106*, 8367.

(2) Selassie, D.; Davis, D.; Dahlin, J.; Feise, E.; Haman, G.; Sholl, D. S.; Kohen, D. *Journal of Physical Chemistry C* **2008**. In press.