Do Coulombic interactions dominate the rate of diffusion of CO_2 and N_2 within all-silica zeolites?

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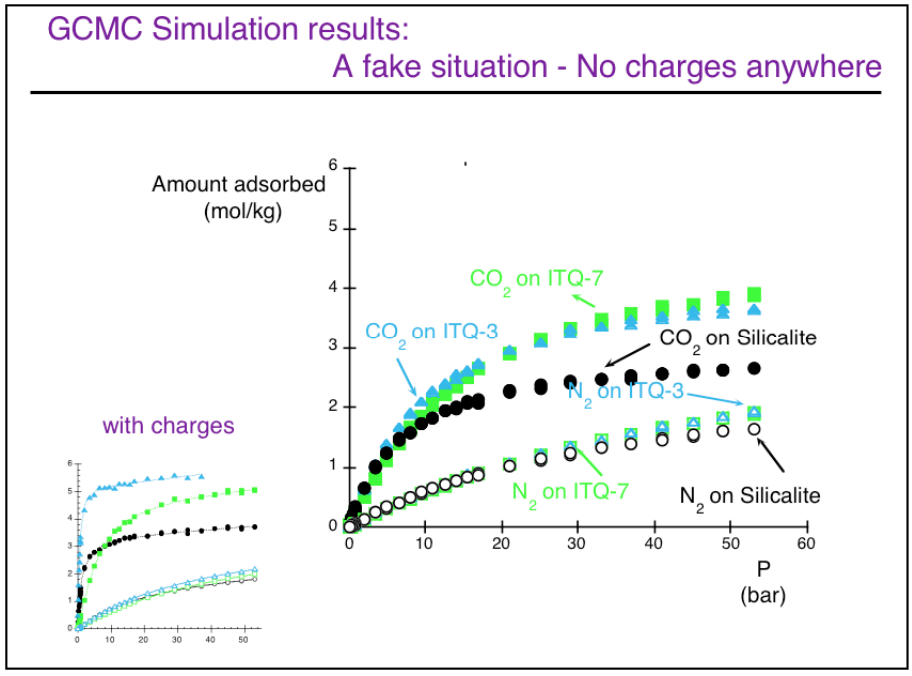
Separation of CO_2 from multi-species gas emissions, such as those found in power plants or cars, requires a filter that is highly selective of CO_2 relative to other non-hazardous components, such as N_2 gas. Zeolites, crystal-structured aluminosilicates, are currently being investigated as promising materials for separation of CO_2 due to their structural diversity and stability.

The behavior of CO_2, N_2 and CO_2/N_2 mixtures within three zeolites with identical chemical composition (SiO_2), but different geometry have been previously studied.[1,2] Grand Canonical Monte Carlo calculations showed that all materials are selective for CO_2 adsorption, but the details depend on the particular structures of the material under study.[1] The calculations also demonstrated that if all coulombic interactions are ignored, the adsorption behavior is dominated by these coulombic interactions (see figure below).

Molecular Dynamic simulations in the same systems show that the diffusion behavior also depends on the material where the gases are diffusing.[2] In the work presented here we describe our efforts to isolate the role of coulombic interactions in this outcome. The role of the coulombic interactions will be studied by comparing diffusion data for simulations with and without coulombic interactions.



(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.