

## How do CO<sub>2</sub> and N<sub>2</sub> molecules orient themselves within the ITQ-3 zeolite?

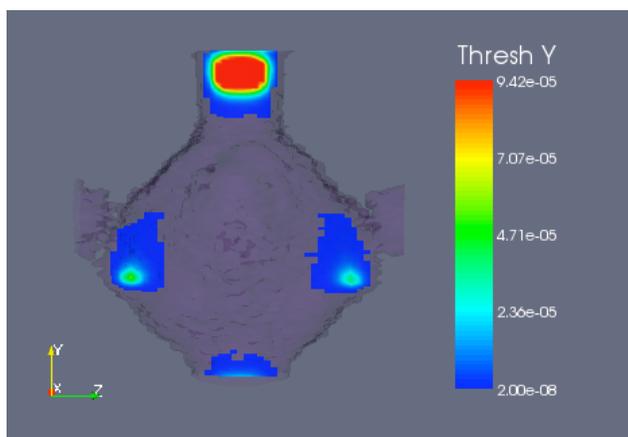
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To efficiently separate CO<sub>2</sub> from multi-species gas streams, sorbents must have high CO<sub>2</sub> selectivity. Zeolites are one attractive option as sorbents due to their variety of structures, availability, and thermal and chemical stability.

We aim to understand and characterize at the molecular level how carbon dioxide and other small gas molecules behave in pores of a variety of zeolites. Using atomistic modeling techniques, we study the adsorption and diffusion processes within zeolites to aid in the identification of adsorbents that are highly selective for CO<sub>2</sub>.

In particular, detailed studies of the siting of N<sub>2</sub> and CO<sub>2</sub> within three zeolites that have the same chemical composition (SiO<sub>2</sub>) but have very different pore structure highlight the importance of preferential adsorption in determining the behavior of mixtures.<sup>1</sup> For example, within ITQ-3 (a material with cages connected by narrow hallways) CO<sub>2</sub> blocks the diffusion of N<sub>2</sub> because CO<sub>2</sub> prefers to occupy the narrow hallways. Note that this behavior is quite unusual and might be important in practical applications.

Previous studies did not address the issue of the orientation of the molecules within the materials' pores, channels and cages. These studies focused on the preferred positions of the center of mass of the adsorbates. The work presented here studies the role of orientation in determining the preferred sites of adsorption. More specifically, we are studying the correlation between molecules' preferred orientations and their potential and free energy.



**Probability map for CO<sub>2</sub> molecules most parallel to the Y-axis within ITQ-3 at 298K.** As shown in red, CO<sub>2</sub> prefers to be parallel to the Y-axis in the narrow hallway in ITQ-3. This hallway is also the most probable location for CO<sub>2</sub> in ITQ-3.

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