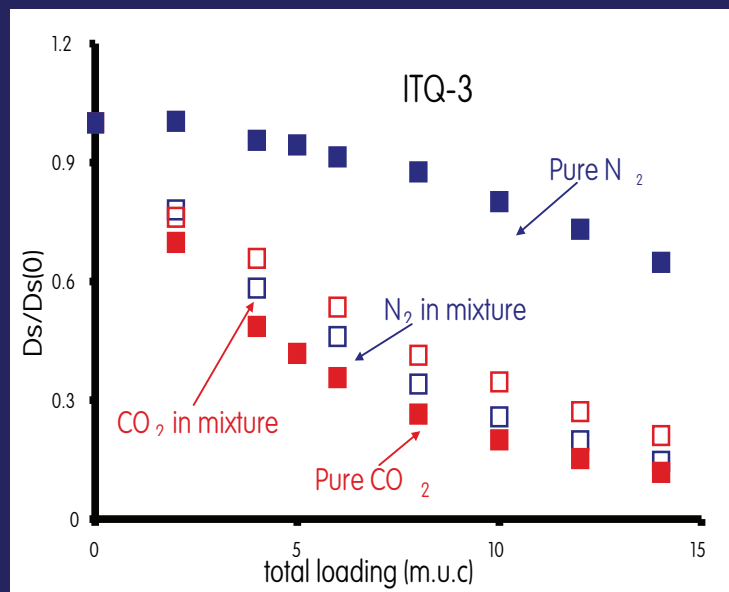


Atomistic Simulations of CO₂ and N₂ in Silica Zeolites: the impact of pore size and shape

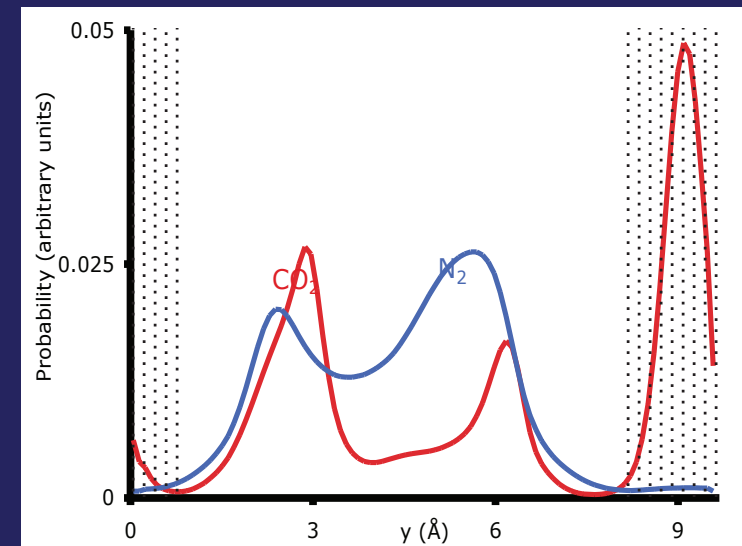
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To efficiently separate CO₂ from multi-species gas streams, sorbents must have high CO₂ selectivity. Zeolites are one attractive option due to their variety of structures, availability, and thermal and chemical stability. We use atomistic modeling techniques to understand and characterize at the molecular level how carbon dioxide and other small gas molecules behave in pores of a variety of zeolites to aid in the identification of adsorbents selective for CO₂.

To investigate the influence of pore geometry on adsorption, selectivity, and diffusion we simulate the behavior of CO₂, N₂ and CO₂/N₂ mixtures within zeolites with identical chemical composition (SiO₂) but different structures. In particular, we have recently shown that gas species move throughout these zeolites at practical speeds, but that the details of the behavior depend greatly on the geometry of the different zeolites.



ITQ-3 is a zeolite with cages connected by narrow channels that very selectively adsorbs CO₂ over N₂. Usually the more mobile species (N₂) is slowed slightly by the less mobile CO₂ and vice versa. This is true within silicalite and ITQ-7 (not shown) but not within ITQ-3.



The preferential sites of adsorption for CO₂ and N₂ are the same within ITQ-7 and silicalite but not within ITQ-3. In ITQ-3, CO₂ molecules preferentially adsorb in the windows that separate the material's cages (shaded regions), whereas for N₂ this is the site of the largest barrier to diffusion. As a consequence CO₂ hinders N₂ diffusion very effectively.