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Gas separation by adsorption in carbon nanohorns.[1] ANTON NEKHAI[2], Rensselaer Polytechnic Institute, SILVINA GATICA, Howard University — Gas separation by adsorption can be accomplished by three basic physical mechanisms: equilibria, kinetics, and steric effects. Equilibrium mechanisms rely on the strength of attraction between gas molecules and their substrate. For example, CO_2 possesses the strongest, attractive interactions with its substrate. As a result, the equilibrium mechanism presents the most plausible strategy to separate carbon dioxide from mixtures. The specification of a sound adsorbent is the key for separation by adsorption. In this paper we investigate carbon nanohrons for selectivity of carbon dioxide over methane. Carbon Nanohorns resemble short, wide, highly defected single-wall nanotubes that end in conical tips ("horns"). In contrast to regular nanotubes that assemble into parallel bundles, nanohorns form spherical aggregates with the nanohorns arranged along radial directions. Using the simulation technique Grand Canonical Monte Carlo (GCMC) we obtained the adsorption isotherms of CH_4 and CO_2 in a 2D array of carbon nanohorns. We estimated the selectivity based on the IAST approximation. We also study the adsorption of argon and neon and compare with experimental results.

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