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Adsorption of ethane in carbon nanostructures[1] JUSTIN PETUCCI, M. MERCEDES CALBI, Physics & Astronomy, University of Denver — We explore the adsorption behavior of ethane on close-ended carbon nanotubes and in as-produced carbon nanohorn aggregates. Adsorption isotherms and isosteric heats of adsorption are obtained by performing Grand Canonical Monte Carlo simulations. Results found for ethane adsorption on the external surface of nanotube bundles are compared with available experimental data and used to build a simple model of adsorption in the more complicated nanohorn structure. Analysis of the equilibrium configurations at increasing pressures provides information about the localization and orientation of the molecules in the different phases that correspond to the steps observed in the experimental and simulated isotherms.

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