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Physisorption Kinetics in Carbon Nanotube Bundles JARED BURDE, M. MERCEDES CALBI, Southern Illinois Univesity, Carbondale — The possibility of adsorbing gases in the interstitial channels that lie between nanotubes in a bundle is still the subject of much discussion because experimental observations do not seem to confirm the existence of adsorbed gases on this site as it has been predicted by several theoretical studies (that assume infinitely long tubes). After exploring the potential energy surfaces near the ends of the tubes, we have recently shown how the presence of a high binding energy site right before the entrance of the channel slows down the adsorption rate of H_2 dramatically [1]. Using a Kinetic Monte Carlo scheme, we present here a comprehensive study of the adsorption kinetics in the channels modeling the transport of various gases through the ends of the bundle. In order to facilitate the comparison with adsorption experiments, the results are given in terms of the equilibration time as a function of coverage, for different temperatures. In addition, the effect of cluster formation at the end of the bundle is analyzed. [1] M. Mercedes Calbi and J. L. Riccardo, *"Energy barriers at the ends of carbon nanotube bundles: Effects on interstitial adsorption kinetics"*, Phys. Rev. Lett. **94**, 246103 1-4 (2005).

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