Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Effects of surface heterogeneity on TPD spectra: a computer simulation study NAYELI ZUNIGA-HANSEN, MERCEDES CALBI, Southern Illinois University — We study gas desorption from external surfaces of carbon nanotube bundles by using a Kinetic Monte Carlo scheme. We focus on desorption of quasi-spherical molecules that form monolayers comprised by three or five lines of molecules along the tubes. Each line is characterized by a particular binding energy. By varying the initial coverage, we observe the effects of this energy heterogeneity of the surface on the Temperature Programmed Desorption Spectra. In particular, by keeping track of the individual coverage on these lines, we investigate the diffusion processes across the lattice and its effect on the spectra. We also discuss implications for available and prospective experimental results.

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Date submitted: 19 Nov 2009 Electronic form version 1.4