Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Temperature Programmed Desorption on Carbon Nanotube Bundles: a Computer Simulation study NAYELI ZUNIGA, MERCEDES CALBI, JARED BURDE, Southern Illinois University Carbondale — We present a study of gas desorption on external surfaces of carbon nanotube bundles by means of a Kinetic Monte Carlo scheme. Starting with an initial coverage, we follow the amount of gas desorbed as the temperature increases for different values of initially occupied sites and initial temperature of the sample. We analyze the spectrum obtained in terms of the different binding energies of the adsorption sites. We also compare our results with some available experimental measurements on nanotube bundles and other nanostructures.

Nayeli Zuniga
Southern Illinois University Carbondale

Date submitted: 26 Nov 2008 Electronic form version 1.4