Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Simulations of adsorption on a single carbon nanotube HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA 70402, SILVINA GATICA, Department of Physics and Astronomy, Howard University, Washington, DC 20059, MILTON COLE, Department of Physics, Pennsylvania State University, State College, PA 16802 — Using the grand canonical Monte Carlo method, we have evaluated the adsorption isotherms of simple gases (Ar, Kr, Xe) on a variety of carbon nanotubes. The adsorption potential is a sum of anisotropic atom-C interactions, dependent on the angle between the outward normal and the atom-C separation vector. For varying gas species and nanotube chirality, different commensurate phases are seen than on the surface of graphite. Comparison is made with recent experiments of Wang, et al, Science 327, 552 (2010).

Hye-Young Kim
Department of Chemistry and Physics,
Southeastern Louisiana University, Hammond, LA 70402

Date submitted: 02 Nov 2010 Electronic form version 1.4