Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Simulations of CO_2 adsorbed on a bundle of carbon nanotubes[1]
MAMADOU MBAYE, SILVINA GATICA, Department of Physics and Astronomy, Howard University, JUSTIN PETRUCCI, MARIA CALBI, Department of Physics and Astronomy, University of Denver — Using the method of grand canonical Monte Carlo (GCMC), we simulated the adsorption of CO_2 in a bundle of closed carbon nanotubes, for temperatures between 74K and 240K. From the outcome of the simulations, we computed the isosteric heat of adsorption, qst. The results are summarized as follows: 1) at low temperature the adsorption isotherms display two steps, which correspond to adsorption in the groove and monolayer completion respectively; 2) at a higher temperature, these steps are smoothed away; 3) at low coverage (up to one monolayer), the qst has the same behavior as for other gases (Ar, Kr) while at higher coverage, it differs from experimental findings. In our simulation the nanotubes were considered smooth, rigid hollow cylinders made of carbon with the density of graphene. The interaction CO_2–NT was computed as the integration of a Lennard-Jones potential plus the CO_2-C quadrupole-quadrupole energy.

[1]This research was supported by ADVANCE/IT (NSF) and NSF (DMR 1006010).

Silvina Gatica
Howard University

Date submitted: 18 Nov 2013 Electronic form version 1.4