Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Adsorption kinetics of polyatomic molecules on a heterogeneous surface JARED T. BURDE, Southern Illinois University Carbondale, M. MERCEDES CALBI, University of Denver — We study the kinetics of adsorption of diatomic and triatomic molecules on the external surface of a carbon nanotube bundle. The Kinetic Monte Carlo algorithm is employed to track the number of particles adsorbed on the bundle and the orientation of those particles with respect to the surface at any given time. Our model is further complicated by the inclusion of a more complex surface geometry; a two dimensional, heterogeneous lattice better models the reality of groove between adjacent nanotubes on the outside of the bundle. This allows us to see interesting kinetic effects in the adsorption process, as the adsorbates have multiple transitional states through which they can pass as they evolve towards equilibrium.

Jared T. Burde
Southern Illinois University Carbondale

Date submitted: 19 Nov 2010 Electronic form version 1.4