



DEPARTMENT OF MECHANICAL ENGINEERING Purdue School of Engineering and Technology

SEMINAR

Date: **Monday, July 11, 2005**

Time: **2:00 pm - 3:00 pm**

Room: **SL 165**

Reception Starts at 1:45 pm. Cookie and Refreshments Served

Monte Carlo Simulation of Hydrogen Adsorption Capacity in Alkali-Doped Single-Wall and Multi-Wall Carbon Nanotubes

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Abstract. Monte Carlo simulations and Widom's test particle insertion method have been used to calculate the solubility coefficients (S) and the adsorption equilibrium constants (K) in single-walled (10,10) armchair carbon nanotubes and multi-wall carbon nanotubes (2-walled and 3-walled) including individual nanotube, and nanotube bundles with various configurations with and without alkali dopants. The hydrogen adsorption isotherms at room temperature were predicted by following the Langmuir adsorption model using the calculated constants S and K . The simulation results were in good agreement with experimental data as well as the Grand Canonical Monte Carlo (GCMC) simulation results reported in the literature. The simulations of nanotube bundle configurations suggest that the gravimetric hydrogen adsorption increases with inter-nanotube gap size. It may be attributed to favorable hydrogen-nanotube interactions outside the nanotubes. The effect of alkali doping on hydrogen adsorption was studied by incorporating K^+ or Li^+ ions into nanotube arrays using a Monte Carlo simulation. The results on hydrogen adsorption isotherms indicate hydrogen adsorption of 3.95 wt% for K-doping, and 4.21 wt% for Li-doping, 4.6 wt% for 2-walled MWNTs and 5.3 wt% for 3-walled MWNTs in reasonable agreement with the experimental results obtained at 100 atm and room temperature (300K). The performances of MWNTs are little better than those of SWNTs.

About the speaker: Xiaoyang Sun is a Master's candidate at Mechanical Engineering Department of IUPUI. He received his bachelor's degree at Tsinghua University, 2003. He is currently a research assistant at Advanced Energy Research Laboratory. His academic advisor is Dr. Hsu, and committee members are Drs. Chen and Akay.