

2008 APS March Meeting
Monday–Friday, March 10–14, 2008; New Orleans, Louisiana

[Session C1: Poster Session I: 2:00 pm - 5:00 pm](#)

2:00 PM–2:00 PM, Monday, March 10, 2008

Morial Convention Center - Exhibit Hall A

Sponsoring Unit: APS

Abstract: C1.00148 : Uptake and isosteric heats of gases adsorbed inside carbon nanotubes

[Preview Abstract](#)

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We studied the properties of gases adsorbed in the interior of open-ended single wall carbon nanotubes for a wide range of pressures and temperatures from tenths to hundreds of Kelvin. The gases studied are Argon, Methane, Hydrogen and Helium in a classical regime. Using the method of Grand Canonical Monte Carlo Simulations we computed the adsorption isotherms, the isosteric heat of adsorption and the configurations at different T,P values. The thresholds values of the pressure and maximum uptake were calculated as a function of the temperature. At the lower temperatures the adsorption of atoms on the axis of the tube is observed as a discontinuous step in the isotherms.