

Abstract Submitted
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Uptake and isosteric heats of gases adsorbed inside carbon nanotubes¹ DANIEL ROBERTSON, SILVINA GATICA, Department of Physics, Howard University — 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.

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Silvina Gatica
Department of Physics, Howard University

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