Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Inelastic Neutron Scattering of H_2 Adsorbed on Boron Doped ($\sim$ 1%) Single Walled Carbon Nanotubes D. NAREHOOD, Department of Physics, The Pennsylvania State University, University Park, PA 16802 USA, Y. LIU, C.M. BROWN, D.A. NEUMANN, National Institute of Standards and Technology, NIST Center for Neutron Research, Gaithersburg, MD 208991, USA, PETER EKLUND, Department of Physics, The Pennsylvania State University, University Park, PA 16802 USA — It is clear from this study that H_2 is preferentially adsorbed at boron sites in SWNTs and in these sites the H_2 experiences an orientational component in the potential. Thus, this study shows that the substitution of boron for carbon in the SWNT lattice produces higher energy binding sites for H_2 adsorption. We report here an inelastic neutron scattering investigation of H_2 adsorbed on $\sim$ 200 mg of purified boron doped ($\leq$ 1%) SWNT bundles. At H_2 coverages $\leq$ 1 H_2/ B and at T = 3K, a clear splitting of $\sim$ 1.4 meV is observed for the sublevels of the J=1 state. As the H_2 coverage is increased, the rotational spectrum converges to that of the bulk like rotor observed for H_2adsorbed on undoped SWNTs with the appearance of a peak at 14.7 meV. As the temperature is increased from 3K, the bulk like peak decreases in intensity until only the split rotational peaks are present; the intensity of these peaks decreases with increasing temperature until about 75 K at which point no rotational peak is observable. Funding provided by the US DOE Office of Energy Efficiency and Renewable Energy within the Center of Excellence on Carbon-based Hydrogen Storage Materials.

Qihua Xiong
Department of Physics, The Pennsylvania State University, University Park, PA 16802 USA

Date submitted: 06 Dec 2005 Electronic form version 1.4