Inelastic Neutron Scattering of H\textsubscript{2} Adsorbed on Boron Doped (~ 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\textsubscript{2} is preferentially adsorbed at boron sites in SWNTs and in these sites the H\textsubscript{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\textsubscript{2} adsorption. We report here an inelastic neutron scattering investigation of H\textsubscript{2} adsorbed on ~ 200 mg of purified boron doped (~ 1%) SWNT bundles. At H\textsubscript{2} coverages ≤ 1 H\textsubscript{2}/ B and at T = 3K, a clear splitting of ~ 1.4 meV is observed for the sublevels of the J=1 state. As the H\textsubscript{2} coverage is increased, the rotational spectrum converges to that of the bulk like rotor observed for H\textsubscript{2} adsorbed 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.

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