Quasielastic Neutron Scattering of H_2 Adsorbed on Single Walled Carbon Nanotubes

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Abstract

From their discovery, carbon nanotubes have drawn interest for a variety of reasons. The attention has been focused on practical applications, such as hydrogen storage and isotope and spin selectivity, to novel effects resulting from the manifestation of reduced dimensionality due to the geometry of the tubes in bundles. Of particular interest is the adsorption and storage of molecular hydrogen in the carbon nanotube bundle due to the possibility of using the nanotubes as a fuel cell for molecular hydrogen. This interest arises from the need for a clean fuel source and a safe and effective method to transport such a fuel. An investigation of the microscopic properties of the adsorbed hydrogen is essential in understanding the suitability for such a system in storing and transporting molecular hydrogen.

We report quasielastic neutron scattering (QENS) measurements performed on molecular hydrogen adsorbed on single walled carbon nanotubes (SWNTs). These measurements indicate that no quasielastic component to the scattering is present below 30K. A quasielastic component is present at 30K, indicating the onset of mobility of the adsorbed hydrogen molecules. This component to the scattering is well described by a liquid-like diffusion model. The observed diffusion is consistent with 2-dimensional diffusion on Grafoil and indicates that the adsorbed hydrogen is leaving the groove sites of the nanotube bundles before diffusing on the outer surface of the bundles.