Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Quasielastic Neutron Scattering of Hydrogen Adsorbed in KC_{24}[1]

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— Quasielastic neutron scattering (QENS) and volumetric techniques were used to study the adsorption of H_2 by the stage-2 potassium graphite intercalation compound KC_{24}. A zero-coverage sorption enthalpy of 8.5 kJ/mol was measured from H_2 isotherms recorded at 77 K and 87 K. The saturation H_2 adsorption amount at 77 K was 1.2 mass%, corresponding to a stoichiometry of $KC_{24}(H_2)_{2.0}$. Quasielastic neutron scattering spectra for $KC_{24}(H_2)_{1.0}$ were collected at temperatures between 40 K and 80 K on a chopper spectrometer and a backscattering spectrometer. Two distinct H_2 diffusion processes were identified with characteristic times of approximately $\tau = 10$ ps and $\tau = 350$ ps at 60 K, respectively. By operating the backscattering spectrometer in fixed window mode, the total elastic scattering of $KC_{24}(H_2)_{1.0}$ was measured as a function of temperature. A sharp decrease in elastic intensity was observed at 35 K due to the onset of quasielastic scattering. This was interpreted as a melting transition of the H_2 adsorbate in KC_{24}.

[1]This work was supported by the Office of Energy Efficiency and Renewable Energy through the Hydrogen Sorption Center of Excellence.

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Date submitted: 20 Nov 2008 Electronic form version 1.4