Properties of molecular hydrogen confined in microporous carbons investigated by neutron spectroscopy techniques

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We report results of vibrational neutron spectroscopy investigation aimed to identify the state of hydrogen adsorbed in ultramicroporous carbon. The mobility of hydrogen confined in carbon pores was probed as a function of temperature and pressure using inelastic neutron scattering, and the molecular translational and rotational motions were studied. At low loading rotation of H_2 molecules adsorbed in the smallest carbon pores (~4–5 Å) is severely hindered, suggesting that the interaction between H_2 and the host matrix is anisotropic. At higher loading, H_2 molecules behave as a nearly free rotor, implying lower anisotropic interactions with adsorption sites. At 77 K where bulk H_2 is a gas, deconvolution of elastic/quasielastic signal provide evidence of pressure-dependent fractions of immobile (solid-like) and partially mobile (liquid-like) hydrogen, which correlate with the excess adsorption isotherm at 77 K. Effective H_2 density in pores changes from solid-like to liquid-like with increasing pressure at 77 K. Surprisingly, immobile and partially mobile H_2 is present even at temperatures as high as ~110 K where bulk hydrogen exists only in gas form. These results correlate well with our previous conclusion on high densification and restricted mobility of H_2 and D_2 confined in carbon nanopores.

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