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Metastable Confinement of Molecular Hydrogen in Double Wall Carbon Nanotubes bundles

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Carbon nanostructured materials are regarded to have high potential for the storage and management of H2 at cryogenic temperatures. We have observed isothermal large hysteretic hydrogen adsorption in samples made out of Double Wall Carbon Nanotubes bundles at 50 K, 77 K and 150 K and up to 15 bar of pressure. Adsorption metastability opens remarkable possibilities: it can be used to lower the working pressure for a given uptake; to increase the usable capacity; or to facilitate thermal management. Metastable H2 adsorption, however, has been barely explored, mostly in the context of Metal-Organic Frameworks (MOFs) [1]. For nanostructured carbons, hysteresis has been associated with chemisorption in metallic particles [3], characterized by undesirably high desorption energy barriers. To gain physical insight, we made a series of inelastic neutron scattering measurements. The elastic signals at different H2 loads are consistent with the uptake of the H2 within the interstitials of the bundles. The quasielastic signal display an anomalous dependence on momentum transfer which is nicely reproduced by an accurate 1D dimensional diffusion model (as expected from interstitial confinement of the H2 fluid) while the complete inelastic signal precludes the possibility of chemisorption onto the sample metallic impurities. We have developed developed a 2D dimensional model that reproduces the qualitative behaviour of the real system. The metastability emerges as consequence of the hierarchical structure of energy barriers, a structure that is sensitive to the H2 uptake through the expansion/contraction of the bundle configuration. Preliminary neutron diffraction results confirm the appearance of this structural hysteresis validating the proposed microscopic mechanisms responsible for the metastability.

1. A. D. P. Broom et al, Applied Physics A, 122 (2016) 151.
2. S. H. Barghi, T. Tsotsis & M. Sahimi, International Journal of Hydrogen Energy, 39 (2014) 1390 .

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