Quasi-elastic neutron scattering for studying the self-diffusion of H_2 adsorbed in carbide-derived carbons for H_2 storage applications

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Porous materials have attracted interest as H_2 storage materials since these can help to alleviate the problem of low storing temperature (20 K) and high storing pressure (300–700 bar) needed to increase the volumetric and gravimetric density of H_2. Namely, the optimal conditions for using porous adsorbents are in the temperature range of 77–150 K and the storage pressure of ~250 bar. The structure of the adsorbent has been shown to have a great impact on the self-diffusion of adsorbed H_2.

Carbide-derived carbons (CDCs) are unique model materials for investigating the impact of the structure of the adsorbents on the H_2 self-diffusion rate and nature since CDCs have a relatively versatile structure. Quasi-elastic neutron scattering (QENS) is a well-suited technique to study the self-diffusion of adsorbed H_2 since neutrons are sensitive towards H_2, neutron energies are suitable to study diffusional processes and neutrons have a large penetration depth allowing *in situ* experiments.

The self-diffusion of H_2 adsorbed in CDCs has been investigated with QENS at temperatures of 20–100 K when the amounts of H_2 adsorbed in CDCs are 2–130 mmol per 1 g of CDC ensuring different pore volume occupancies. The self-diffusion of adsorbed H_2 is shown to occur over multiple timescales (Figure 1) and the confinement of the adsorbed H_2 depends on the pore wall corrugation, i.e., the volume of ultramicropores[1] (pore width $w < 7$ Å). The self-diffusion of H_2 adsorbed in ultramicropores is shown to be very restricted (Figure 1a) and rotational[2]. When adsorbed in larger pores, i.e., micro- ($w < 20$ Å) and mesopores (20 Å $< w <$ 500 Å), the adsorbed H_2 is more mobile (Figure 1b) and the self-diffusion mechanism is translational[2]. Such distinction between components of adsorbed H_2 are only possible to be made by applying QENS over a wide temporal range and these results provide valuable insight into the nature of H_2 self-diffusional dynamics and structure of adsorbents for cryo-adsorptive system development.

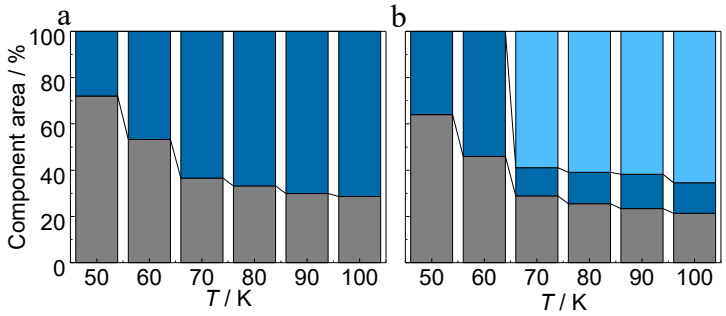

Figure 1: Effectively immobile (gray), mobile (dark blue), and very mobile (light blue) fractions of H_2 adsorbed in a) ultramicropores (4 mmol g^{-1}) and b) micropores (21 mmol g^{-1}) of a CDC from QENS.

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References
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