

Contribution ID: 41 Contribution code: **Board 23**Type: **Poster Presentation**

Small-angle neutron scattering reveals high-density adsorbed hydrogen in carbon micropores at low pressures and supercritical temperature

Monday, May 20, 2024 7:10 PM (20 minutes)

This study reports on the low-pressure supercritical Hydrogen (H₂) and Deuterium (D₂) adsorption in a nanoporous activated carbon cloth, investigated by small-angle neutron scattering (SANS) to elucidate pore size dependent adsorbate densification [1]. The changes of the SANS signal resulting from the physisorption of adsorbate molecules in the pore space are described by analytical pore scattering functions resembling slit-like pores. Based on a hierarchical pore model, we are able to quantify the pore-size-dependent physical density of the confined gas for three pore classes, resembling roughly the IUPAC classes of ultramicropores, supermicropores, and mesopores. Within the very smallest pores, we find the adsorbate density of both, H₂ and D₂, approaching the bulk solid density of the adsorbate for pressures of about 1 bar at 77 K, while the adsorbate density remains much lower for larger pores. The implications of these results for the design of optimized carbons for low pressure / high temperature hydrogen adsorption are discussed. Moreover, the limitations of the approach and possible ways of overcoming them are also critically reviewed.

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Session Classification: Poster Session

Track Classification: Poster Presentations