Hydrogen Physisorption Mechanisms in Nanoporous Carbons:

Insights from Small Angle Neutron Scattering using a Hierarchical Contrast Model

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Motivation

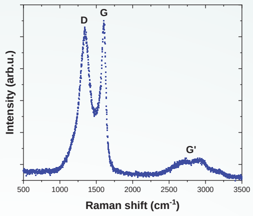
Hydrogen will play an important role in the transition from a fossil fuel based economy towards a renewable and CO_2 free one in the future. The hydrogen needed in industrial applications, such as steel making [1], can be stored in large high pressure storage vessels or underground caverns, whereas mobile hydrogen storage solutions for fuel cell electric vehicle require a volume-efficient and light weight structure [2]. The hydrogen storage performance of high surface area activated carbons at cryogenic temperatures offers a possible solution. In order to enhance the performance, an understanding of the basic physical processes of the solid-gas interaction is crucial. Within this work we try to elucidate the effects of pore size and pressure on the density evolution of the confined hydrogen using Small Angle Neutron Scattering and the insights from a hierarchical contrast model.

Materials characterization

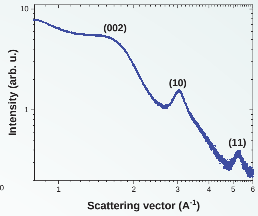
Thorough materials characterization enables us to understand the structure of the material from a macroscopic scale down to the atomistic scale.

Gas Sorption Analysis is a fast an non-destructive technique, which elucidates the pore structure, the surface area as well as the pore volume [3].
Raman spectroscopy and X-ray diffraction helps to understand the atomistic structure of the material [4].
X-ray photoelectron spectroscopy is a powerful tool to asses the chemical composition of the activated carbon [5] .

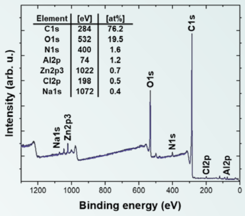
Raman



XRD

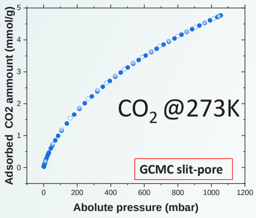


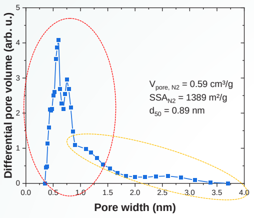
XPS

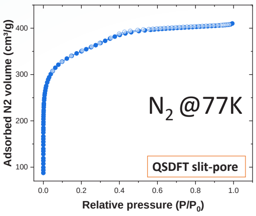


Element	[eV]	[at%]
C1s	284	76.2
O1s	532	19.5
N1s	400	1.6
Al2p	74	1.2
Zn2p3	1022	0.7
Cl2p	198	0.5
Na1s	1072	0.4

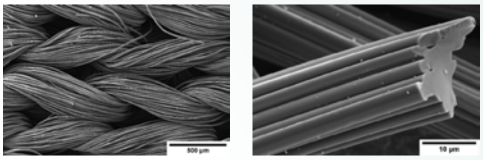
Gas Adsorption







Scanning electron microscopy



Combining Gas Adsorption and Small Angle Neutron Scattering

Small momentum transfer diffractometer D16@ILL

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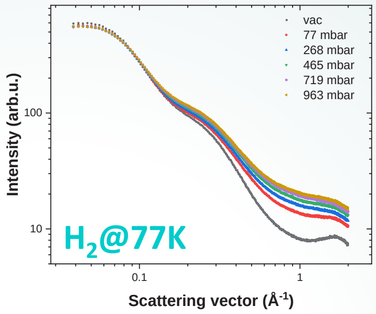

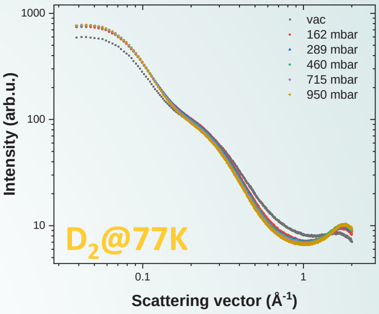

The hierarchical pore scattering contrast model

$$I_{(q)pore} = \frac{S_{d(p)} \cdot T^2}{\tilde{I} \cdot q^2} \cdot \left[\frac{(qT)^2 + (a-1)\cdot(a^2+b^2)}{\left((qT)^2 + a^2 - b^2\right)^2 + 4a^2b^2}\right]$$

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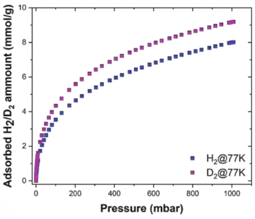
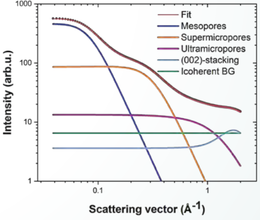
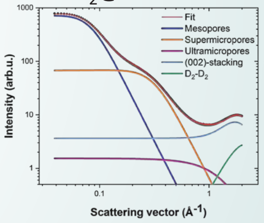


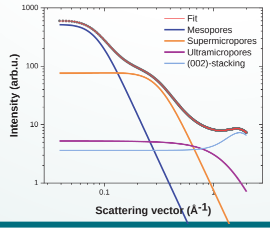
H$_2$@963 mbar



D$_2$@950 mbar



Sample@vacuum



$$\frac{S_{d(p)}}{S_{d(0)}} = \frac{\varphi_d \cdot \varphi_{matrix} \cdot \left(\langle\tilde{\rho}_{matrix}\rangle - \tilde{\rho}_d\right)^2}{\varphi_d \cdot \varphi_{matrix} \cdot \langle\tilde{\rho}_c\rangle}$$

$$\rho_{gas} = \frac{M_{H2/D2} \cdot \tilde{\rho}_d}{b_{H2/D2} \cdot N_A}\left(\frac{\mathrm{g}}{\mathrm{cm}^3}\right)$$

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References

[1] D. Ernst, et. al., Plasma Smelting Reduction Process, (2023). Metals 2023, 13(3), 558; https://doi.org/10.3390/met13030558
[2] D.P. Broom, D. Book, Hydrogen storage in nanoporous materials, in: Adv. Hydrog. Prod. Storage Distrib., Elsevier Inc., 2014: pp. 410–450. https://doi.org/10.1533/9780857097736.3.410.
[3] M. Thommes, et. al., Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution (IUPAC Technical Report), Pure Appl. Chem. 87 (2015) 1051–1069. https://doi.org/10.1515/pac-2014-1117.
[4] S. Stock, et. al., Coffee Waste-Derived Nanoporous Carbons for Hydrogen Storage, ACS Appl. Energy Mater. (2022). https://doi.org/10.1021/acsaem.2c01573.
[5] N. Kostoglou, et. al., Nanoporous activated carbon cloth as a versatile material for hydrogen adsorption , selective gas separation and electrochemical energy storage, Nano Energy (2017), https://doi.org/10.1016/j.nanoen.2017.07.056.

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