In situ small-angle neutron scattering study of hydrogen physisorption in nanoporous carbons

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MONTAN UNIVERSITÄT LEOBEN

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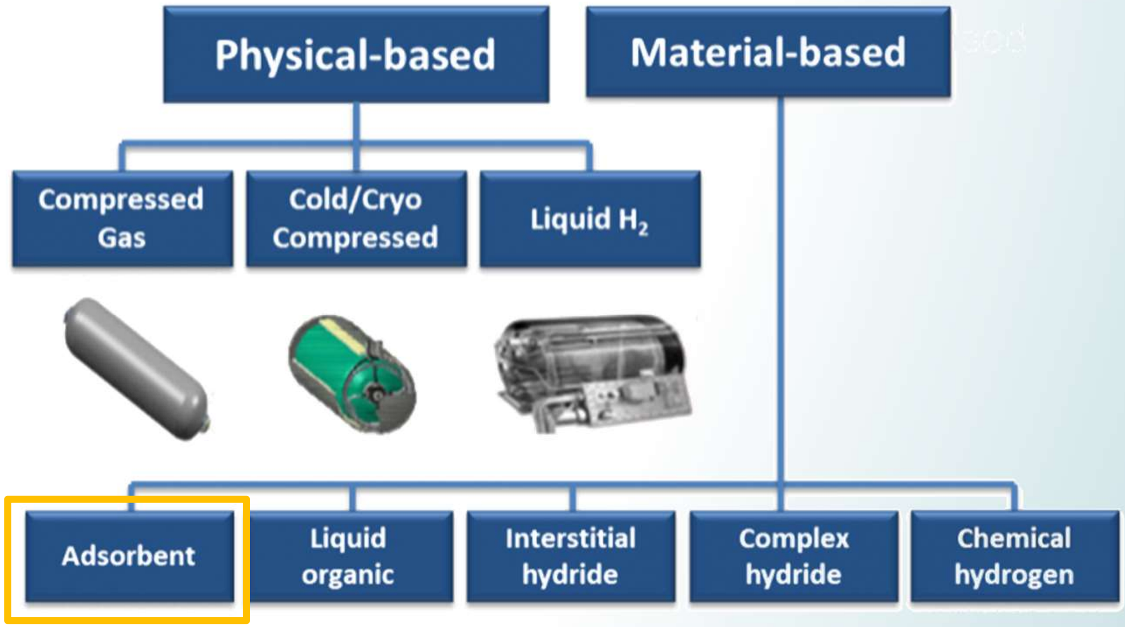
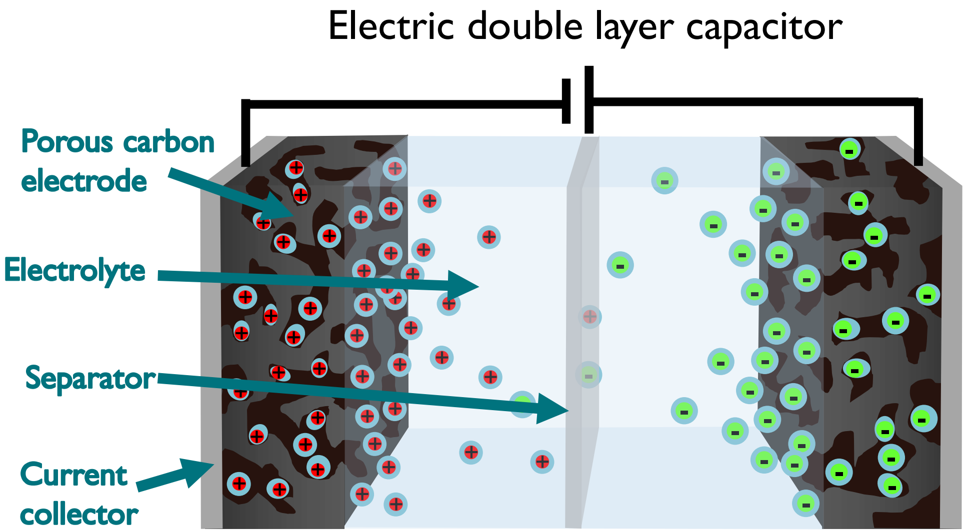
How to storage H_2

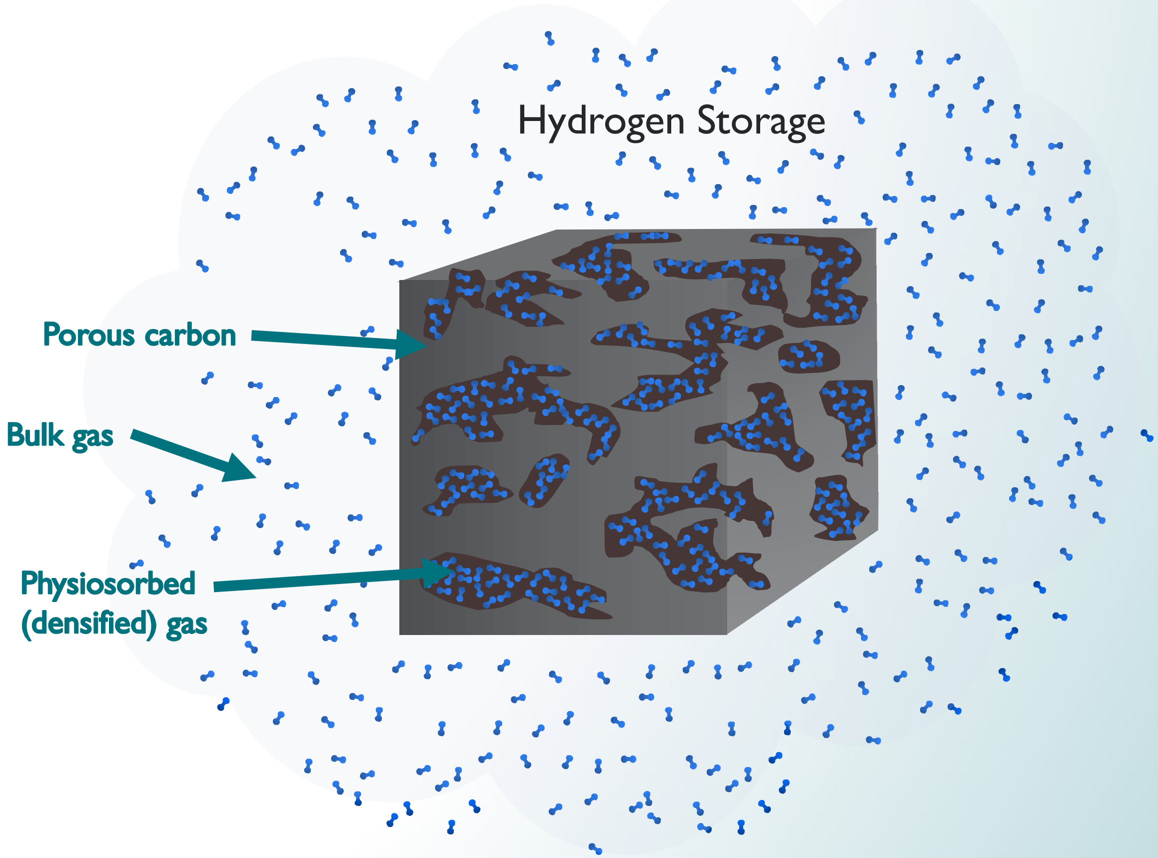
- Pressure and temperature:
  - Compression up to 700 bar
  - Liquefaction of H_2 at 20.3 K
  - Cooling + compression
- Interaction with other materials:
  - Physical interaction: adsorption
  - Chemical interaction: absorption



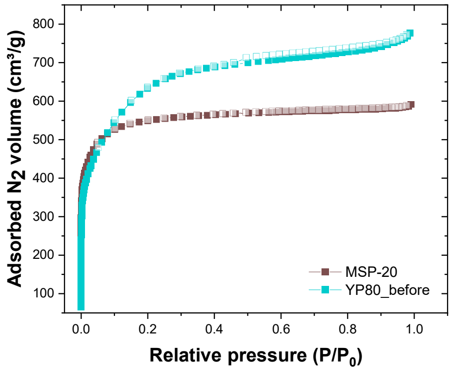
https://www.energy.gov/eere/fuelcells/hydrogen-storage

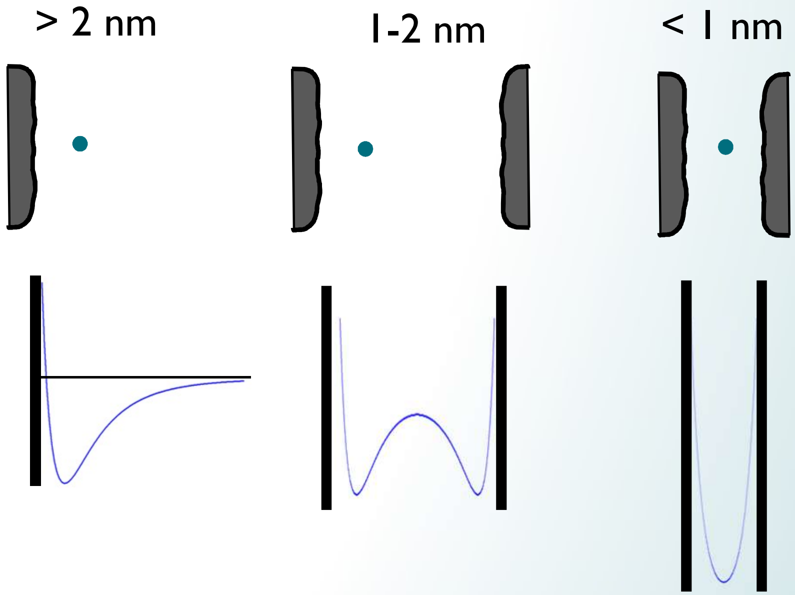
Introduction – Why nanoporous Carbons?

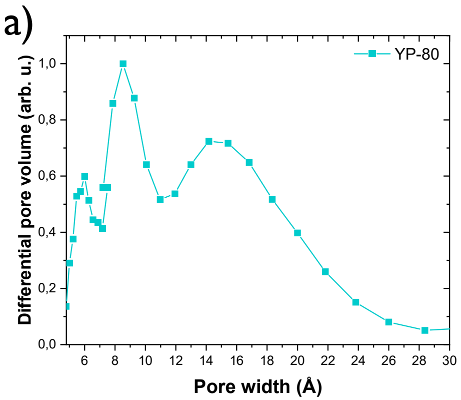


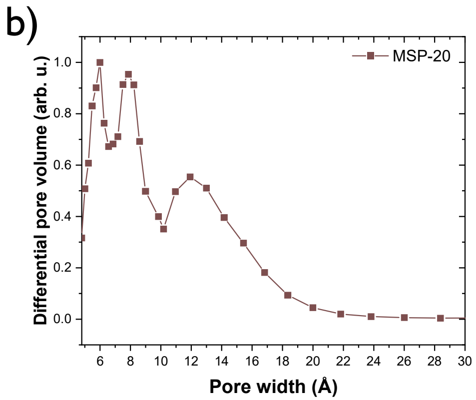


What is important for H_2 storage?



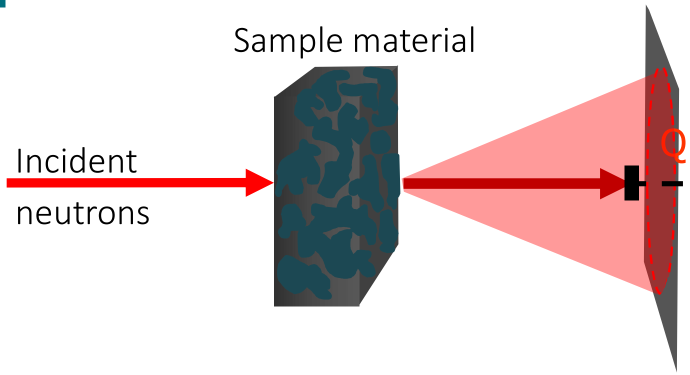


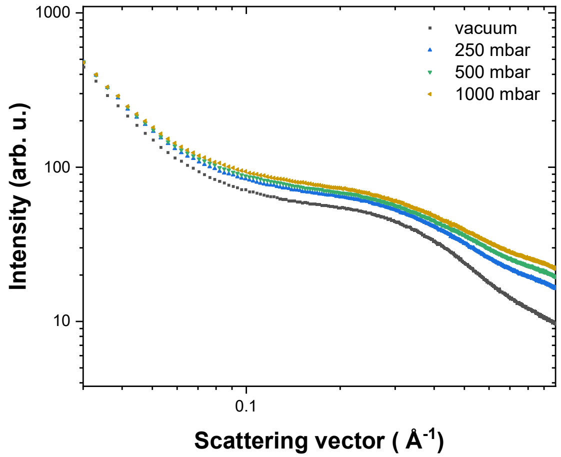




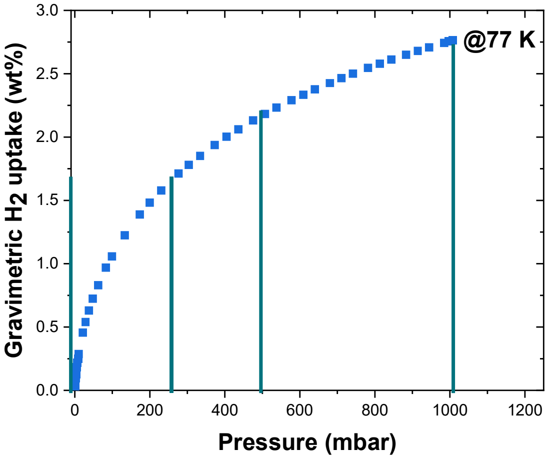
- Specific surface area
- Specific pore volume
- Pore size distribution
- Surface functionalities

What do we want to know?



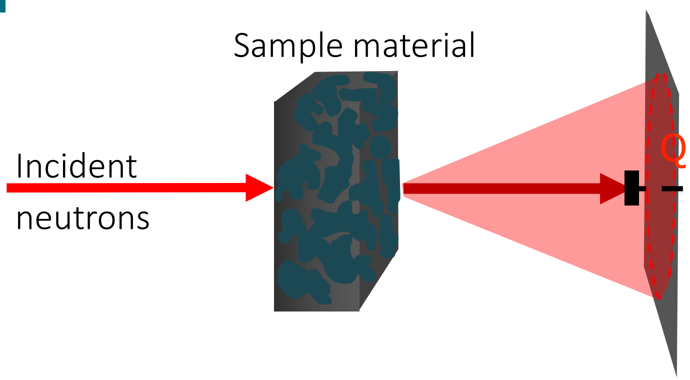


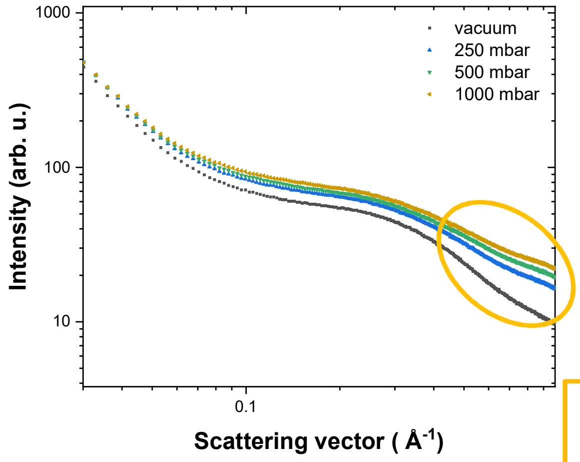
Small momentum transfer diffractometer D16 @ILL



- How does the pore size influence the gas density?
- How does the pore shape influence the uptake?
- What are the optimal pore size and shape characteristics for highest adsorption?

Gas density from SANS – Two-phase model approach



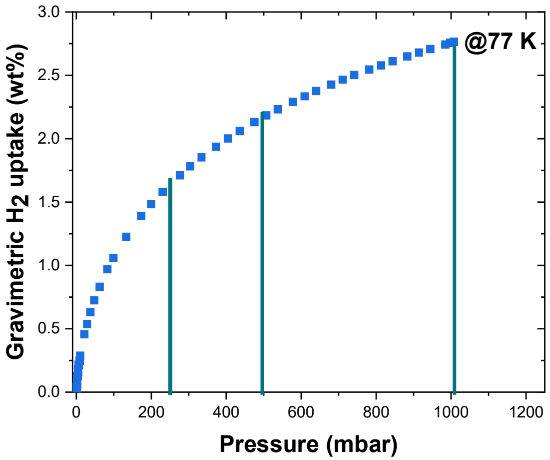


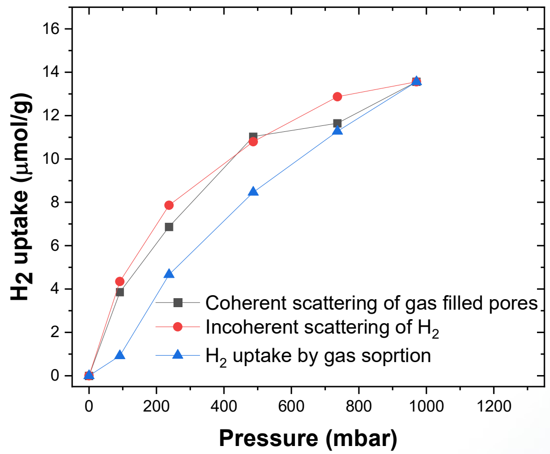
$$I_{(Q)} = I_{particle} + I_{pore} + I_{fluct}$$

$$\lim_{Q\to\infty} I_{pore} = B * Q^{-k} + I_{fluct} + I_{inc}$$

$$k = 4 \; sharp \; interfaces$$
$$k < 4 \; non - \; sharp \; interfaces$$

$$I_{inc} \propto \left(\frac{b_{H2,inc} \cdot N_A}{M_{H2}} \cdot \rho_{H2} \right)^2 \propto \frac{M_{H2} * uptake}{V_{pore}}$$





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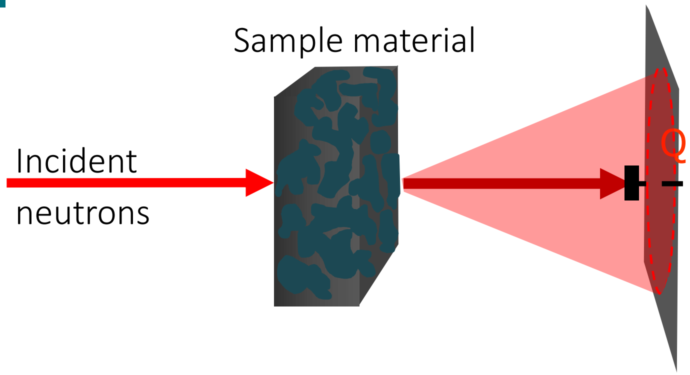

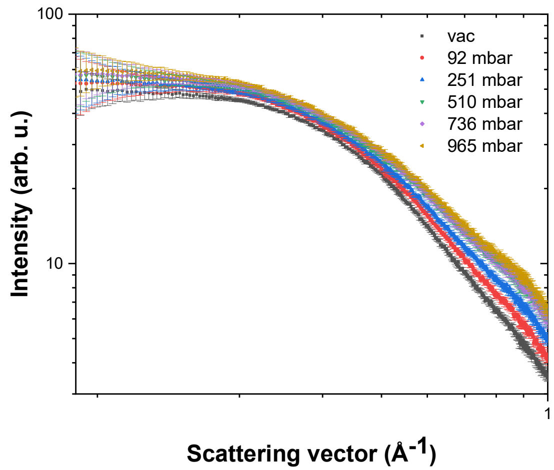

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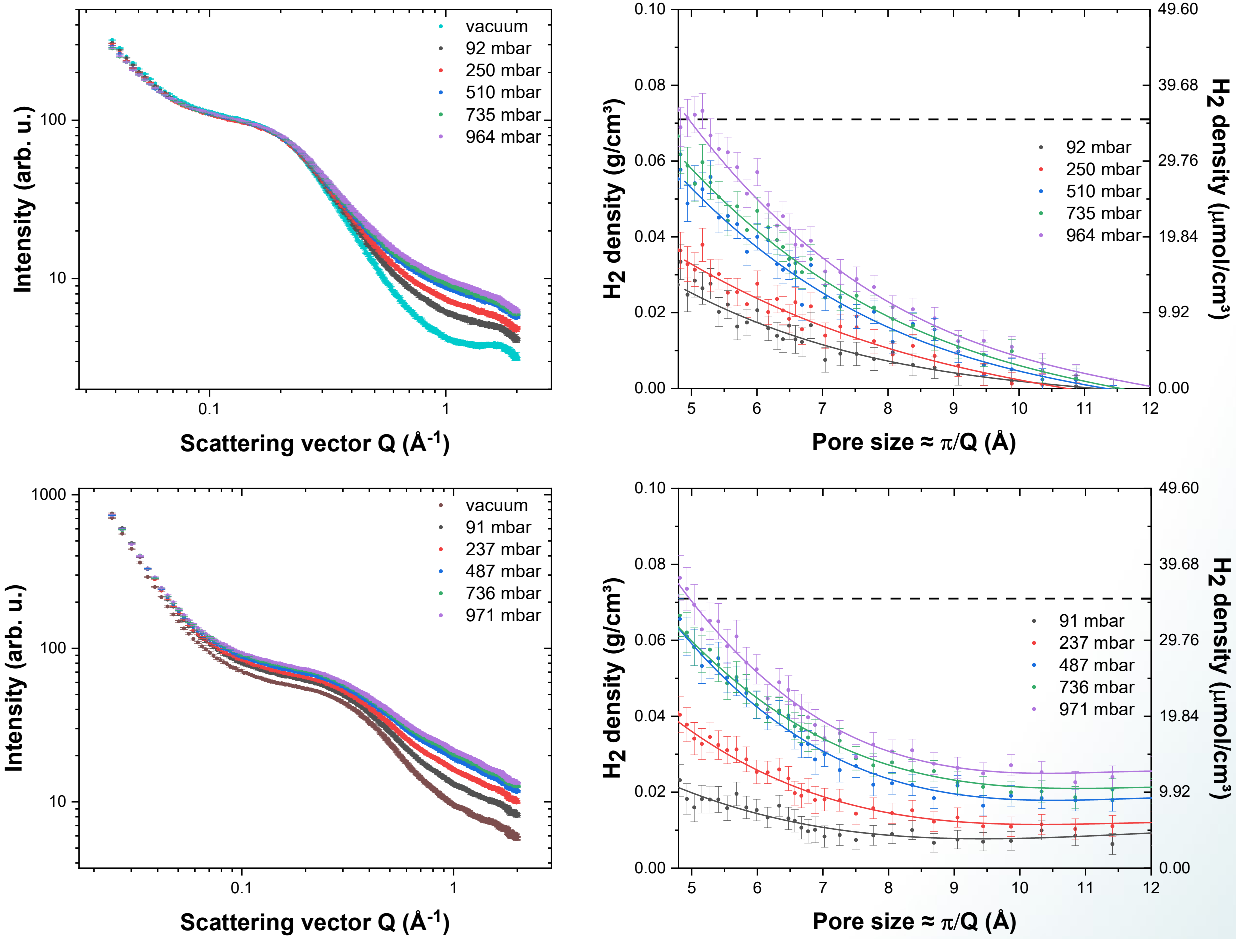
Element	b_{coh} (10^{-13} cm)	b_{inc} (10^{-13} cm)
C	6.65	0
H_2	-7.48	25.27
D_2	13.34	4.04

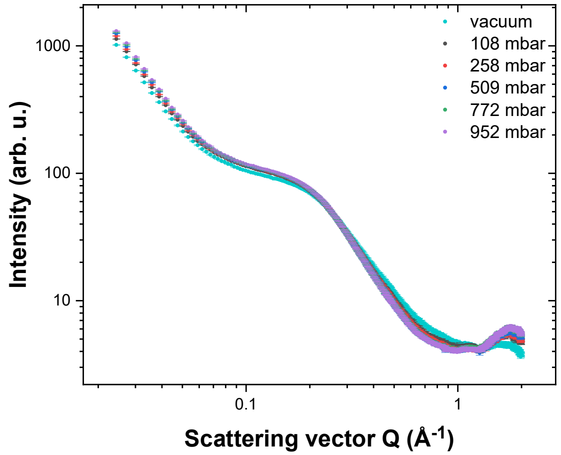
$$\rho_{(Q),H2/D2} = \frac{b_c \cdot M_{H2/D2} \cdot \rho_C}{b_{H2/D2} \cdot M_C} \cdot \left(1 - \sqrt{\frac{I_{(Q,P),coh}}{I_{(P=0),coh}}}\right)$$

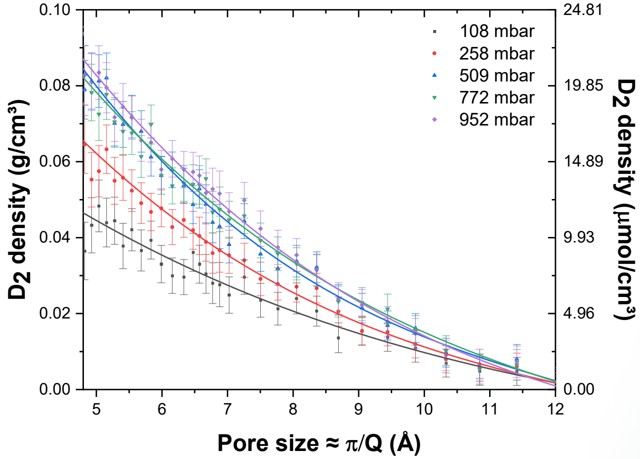
(Gallego et. al., 2011)

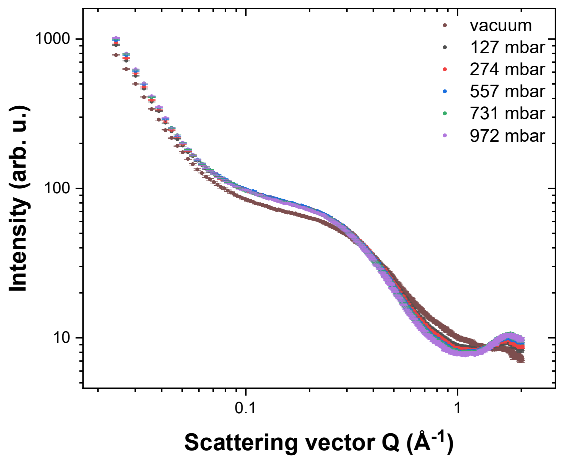
H_2 physisorption

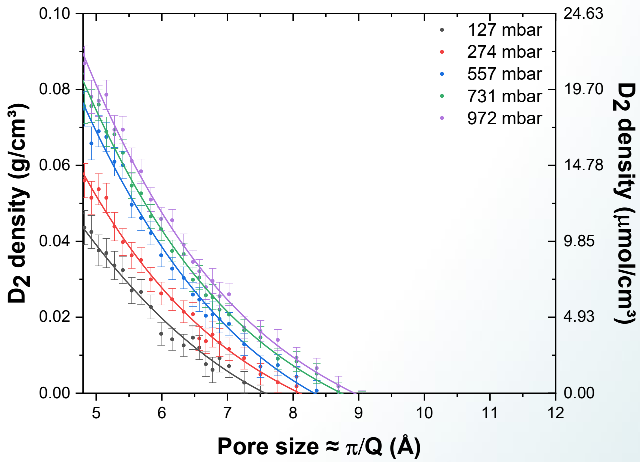


D_2 physisorption



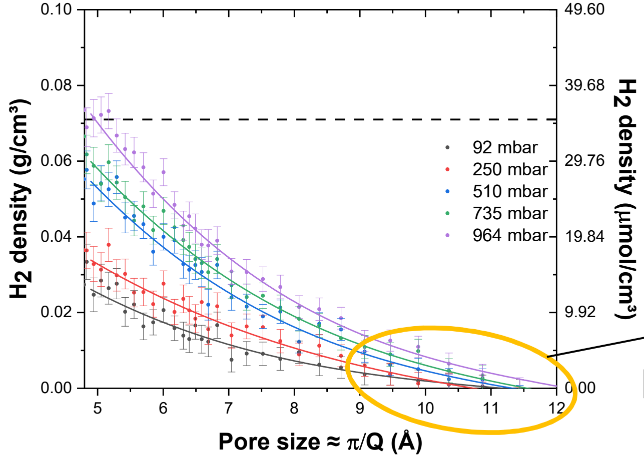




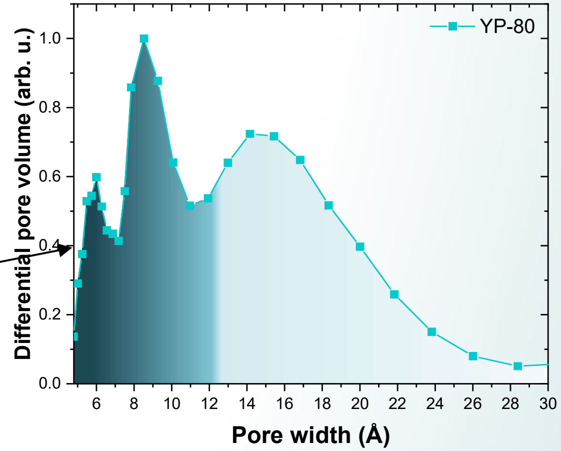


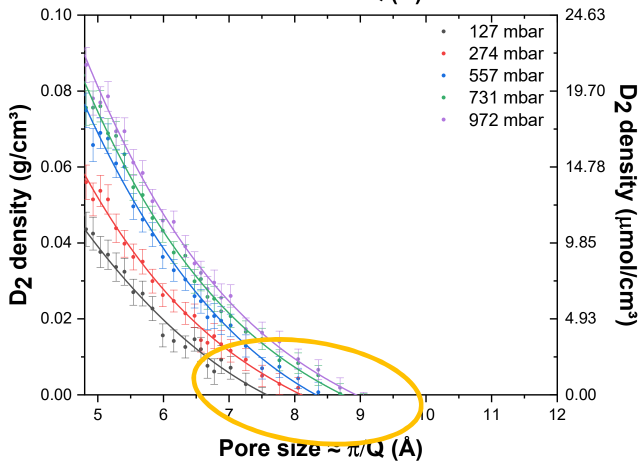
What can we learn?

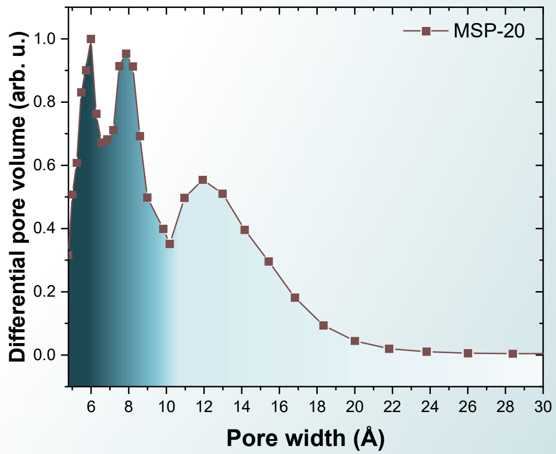
$$\rho_{(Q),H2/D2} = \frac{b_C \cdot M_{H2/D2} \cdot \rho_C}{b_{H2/D2} \cdot M_C} \cdot \left(1 - \sqrt{\frac{I_{(Q,P),coh}}{I_{(P=0),coh}}}\right)$$



Fractional pore filling







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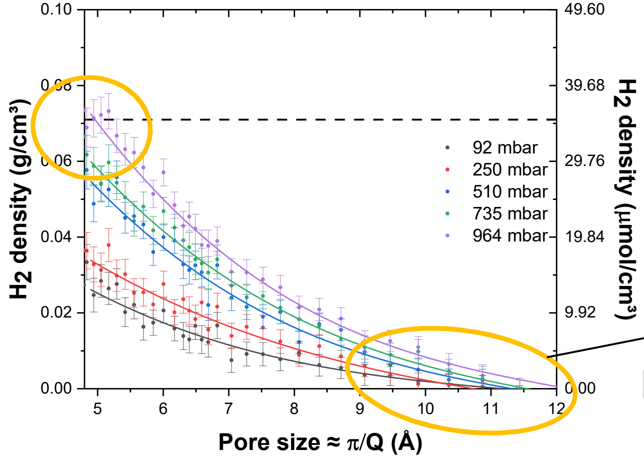

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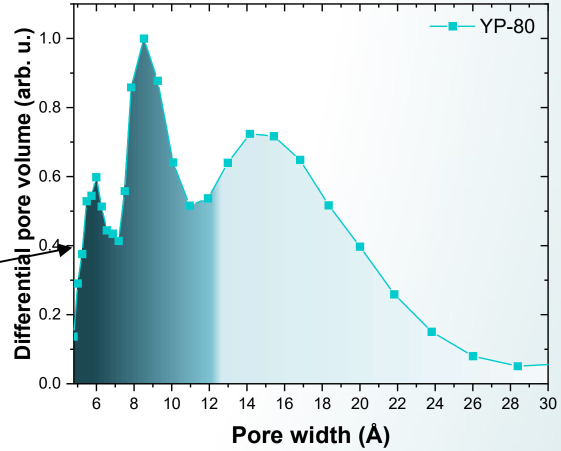

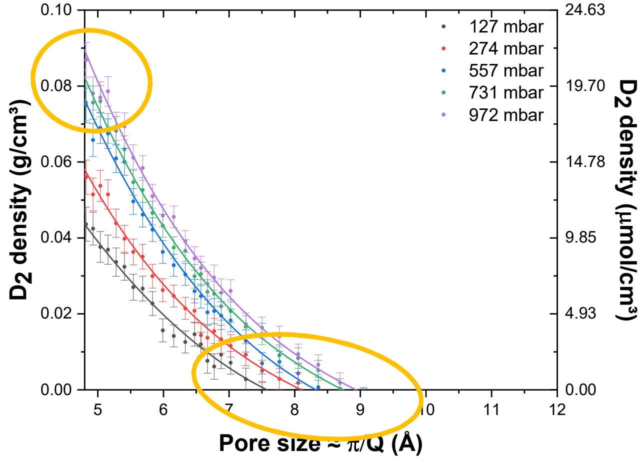

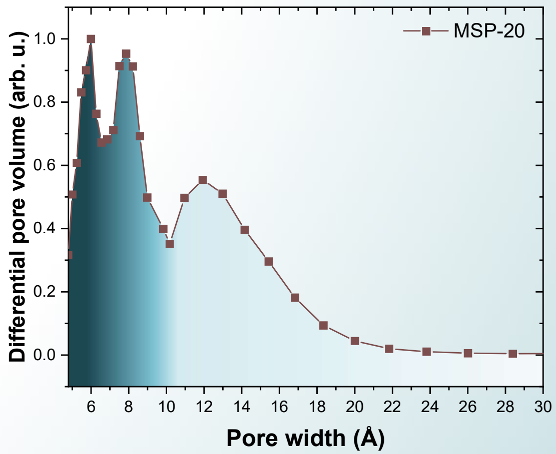

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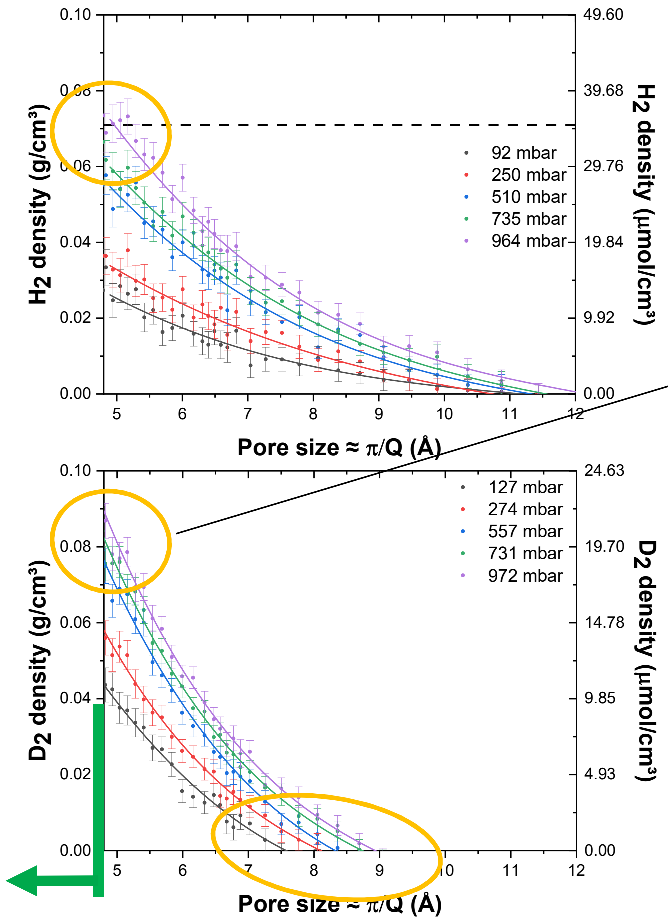

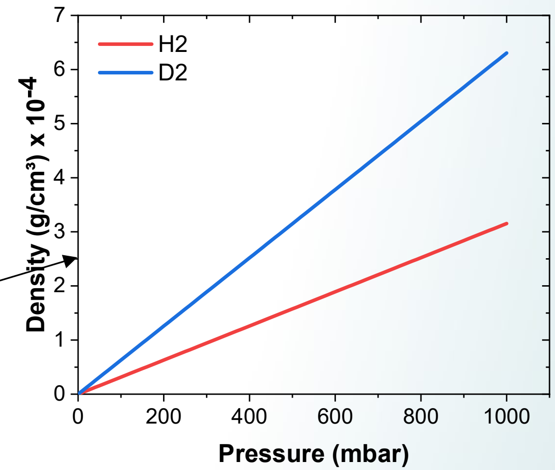

Quantum effects – Thermal wavelength:

$$\lambda = \frac{h}{\sqrt{2\pi \cdot m \cdot \ _B \cdot T}}$$

$$\lambda_{H2} = 1.76\ \text{Å}$$

$$\lambda_{D2} = 1.24\ \text{Å}$$

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Carbon 173 (2021) 968–979

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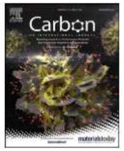

Research Article

Effect of pore geometry on ultra-densified hydrogen in microporous carbons

Mi Tian [a, b, *], Matthew J. Lennox [b], Alexander J. O'Malley [c], Alexander J. Porter [c], Benjamin Krüner [d, e], Svemir Rudić [f], Timothy J. Mays [b], Tina Düren [b], Volker Presser [d, e], Lui R. Terry [g], Stephane Rols [h], Yanan Fang [i], Zhili Dong [i], Sebastien Rochat [j], Valeska P. Ting [g, **]

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Inelastic neutron scattering

Carbon 197 (2022) 359–367

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Miriam Koppel [a], Rasmus Palm [b, *], Riinu Härmas [a], Margarita Russina [c], Veronika Grzimek [c], Jacek Jagiello [d], Maarja Paalo [a], Heisi Kurig [a], Martin Månsson [b], Ove Oll [a], Enn Lust [a]

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Quasi-elastic neutron scattering
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https://doi.org/10.1038/s41557-022-01019-7

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Rafael Balderas-Xicohténcatl [1,2]✉, Hung-Hsuan Lin[3], Christian Lurz[3], Luke Daemen[2], Yongqiang Cheng[2], Katie Cychosz Struckhoff[4], Remy Guillet-Nicolas[5], Gisela Schütz[1], Thomas Heine [3,6,7], Anibal J. Ramirez-Cuesta [2], Matthias Thommes[8] and Michael Hirscher [1]✉

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Manipulation of the crystalline phase diagram of hydrogen through nanoscale confinement effects in porous carbons†

Lui R. Terry, [*a] Stephane Rols, [b] Mi Tian, [c] Ivan da Silva, [d] Simon J. Bending [e] and Valeska P. Ting [*a]

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Bruno Demé (Co-Supervisor)
Viviana Cristiglio
Olivier Aguettaz

Mark Baker and his team (XPS)

Christian Prehal (Discussions)

Volker Presser and his team (CHNS-O)