Bristol Composites Institute (ACCIS)

ACCIS — Advanced Composites Collaboration for Innovation & Science

UKRI Engineering and Physical Sciences Research Council

University of Bristol — EPSRC Centre for Doctoral Training in Composites Science, Engineering and Manufacturing

Semi-empirical Modelling of Hydrogen Sorption Isotherms

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Solid-state hydrogen storage is the **key to environmentally -friendly fuel economy**. Several reports have demonstrated adsorption within **micropores can densify hydrogen past the solid phase** [1] moving the field closer to practical hydrogen storage. However, determination of adsorbate hydrogen density is **difficult, expensive and time -consuming**. Semi-empirical modelling can provide an estimate of density from gas sorption isotherms. To simplify/automate this process, two MATLAB functions were developed to calculate the adsorbate density and heat of adsorption directly from gas sorption data. These were used to identify material properties leading to greater hydrogen density to facilitate the rational design of **microporous carbon materials for nano -composite hydrogen storage vessels**.

Fitting of Experimental Hydrogen Uptakes

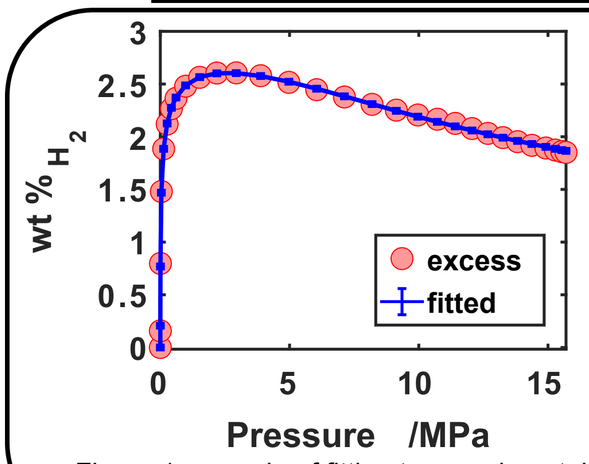
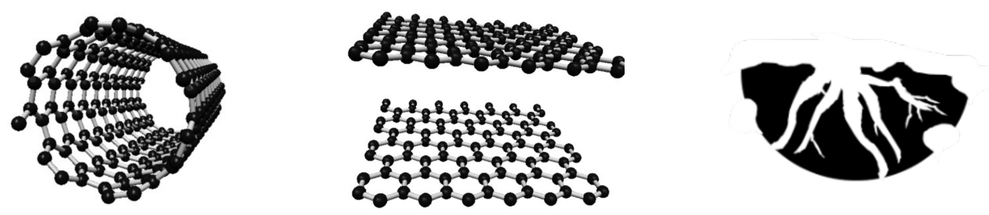


Figure 1 example of fitting to experimental data using the MATLAB function

( )
- Adsorbate Density
- Bulk Density
- Pore Volume
- Fill Volume Fraction

Improved data handling
In-built hydrogen data
Increased automation
Inexpensive

Porous Carbon Materials



Material (pore geometry)	BET SSA /$m^2.g^{-1}$	Total V_p /$cm^3.g^{-1}$	Pore Size /nm
SWCNTs (cylindrical)	945	0.89	0.58, 0.95 and 1.16
TiC -CDC (slit)	1107	0.46	0.66
TE7 (disordered)	1234	1.33	0.68, 1.2 and 1.5
AX21 (disordered)	2524	1.82	1.3 and 1.5 -5

Calculation of Isosteric Heat of Adsorption

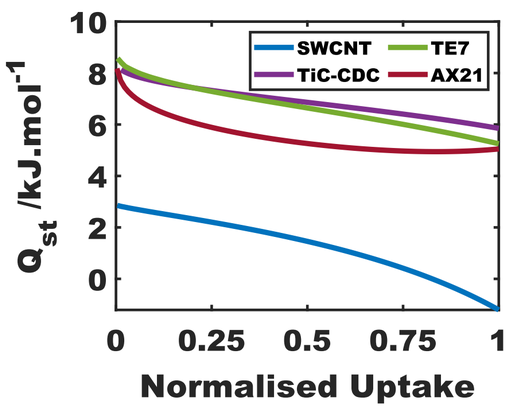


Figure 2 Calculated isosteric heat of adsorption with increasing H_2 uptake

What?
The heat released upon H_2 binding to the surface

Why?
Indicates how strongly bound H_2 is to the surface

How?
Fitting and extrapolation of isotherm data across different temperatures

Results

Higher Heat of Adsorption = Higher Density

Disordered porous networks beneficial for Hydrogen densification

More micropores (< 2 nm) and ultra-micropores (< 0.7 nm) better for densification

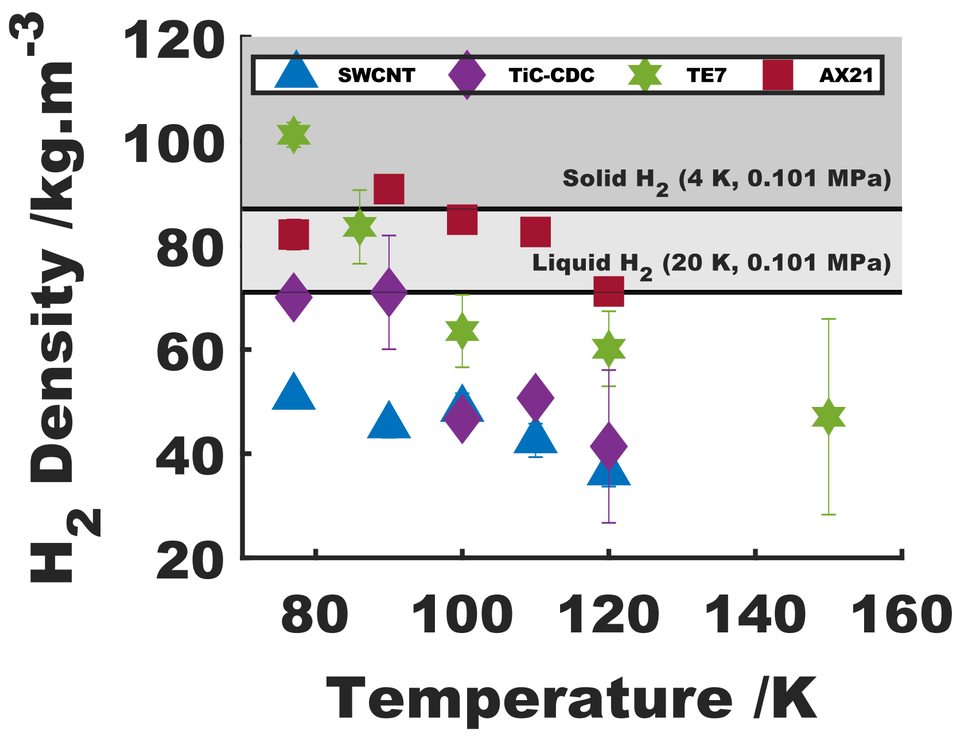


Figure 3 Plot showing the effect of temperature versus adsorbate density determined through used of the MATLAB (AX21 90-120 K inclusive are taken from Bimbo et al.)[2]

Conclusion

Fitting function adequately fits all data for all materials at any temperature

Values from fitting can be passed directly to the second function to calculate the heat of adsorption

Chemical modification or optimisation of pore geometry may increase heat of adsorption

References

1. Ting VP, Ramirez-Cuesta AJ, Bimbo N, Sharpe JE, Noguera-Diaz A, Presser V, et al. Direct evidence for solid-like hydrogen in a nanoporous carbon hydrogen storage material at supercritical temperatures. ACS nano. 2015;9(8):8249-54.
2. Bimbo, N., et al., *Isosteric enthalpies for hydrogen adsorbed on nanoporous materials at high pressures.* Adsorption, 2014. **20**(2-3): p. 373-384.