Contribution ID: **25** Type: **Oral**

Nanoconfining H2 - manipulation of the phase diagram and consequences of reduced freedom

Wednesday, 14 September 2022 15:35 (35 minutes)

Condensed phases of molecular hydrogen (H2) are highly desired for clean energy applications ranging from hydrogen storage to nuclear fusion and superconductive energy storage. However, in bulk hydrogen, such dense phases typically only form at exceedingly low temperatures or extremely high (typically hundreds of GPa) pressures, reducing accessibility of application.

Formation of solid-like H2 at atmospheric pressure at temperatures above the critical point has been indicated in when H2 is confined in nanoscale pores of carbon nanomaterials indicating an alternative route to access condensed phased at more accessible pressures and temperatures.1–3

To understand the potential of nanoconfinement for manipulation of the hydrogen phase diagram, we explore which H2 solids form and why when confined inside carbonaceous nanoscale pores, and investigating pore size and geometry effects.

Using a powerful combination of variable temperature and variable pressure inelastic neutron scattering and neutron diffraction we study the rotational dynamics, distribution and arrangement and structure of nanoconfined H2.4,5

Our results lead us to a general strategy for further manipulation of the H2 phase diagram via nanoconfinement effects, and for tuning of anisotropic potential through control of confining material composition and pore size.

References

1. Ting, V. P. et al. Direct Evidence for Solid-like Hydrogen in a Nanoporous Carbon Hydrogen Storage Material at Supercritical Temperatures. ACS Nano 9, 8249–8254 (2015).

2. Gallego, N. C., He, L., Saha, D., Contescu, C. I. & Melnichenko, Y. B. Hydrogen Confinement in Carbon Nanopores: Extreme Densification at Ambient Temperature. J. Am. Chem. Soc. 133, 13794–13797 (2011).

3. Olsen, R. J. et al. Phase Transition of H2 in Subnanometer Pores Observed at 75 K. ACS Nano 11, 11617–11631 (2017).

4. Terry, L. R. et al. Manipulation of the crystalline phase diagram of hydrogen through nanoscale confinement effects in porous carbons. Nanoscale 14, 7250–7261 (2022).

5. Tian, M. et al. Effect of pore geometry on ultra-densified hydrogen in microporous carbons. Carbon N. Y. 173, 968–979 (2021).

Primary author: Dr TERRY, Lui

Co-authors: Prof. TING, Valeska (University of Bristol); Dr ROLS, Stephane (ILL); Dr DA SILVE, Ivan (ISIS); Dr TIAN, Mi (University of Exeter); Prof. BENDING, Simon (University of Bath)

Presenter: Dr TERRY, Lui

Session Classification: Session 5 : Catalysis & Pourous materials II