Effects of nanoscale confinement on hydrogen in porous carbons

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High surface area nanoporous materials such as porous carbons, zeolites and metal-organic frameworks are exceptionally suited for applications in gas separation and storage. Their nanoscale structures can be tuned to allow exceptionally high densities of gas within their pores \cite{1}, which can lead to exciting possibilities for energy storage, both by physical adsorption of alternative fuel gases such as hydrogen and through emergence of unusual materials states via gas densification.

In bulk hydrogen, such dense phases typically only form at exceedingly low temperatures or extremely high (typically hundreds of GPa) pressures. However, confinement of H\textsubscript{2} within nanoporous materials has been shown to significantly manipulate the hydrogen phase diagram leading to preferential stabilization of unusual crystalline H\textsubscript{2} phases.

We used pressure and temperature-dependent neutron scattering to map out the phase diagram of H\textsubscript{2} when confined inside both meso- and microporous carbons, demonstrating stabilisation of crystalline hydrogen in microporous carbons, at temperatures far higher than would be possible in bulk H\textsubscript{2} \cite{2}. Such nanoconfinement effects could potentially provide lower energy routes to the formation and study of more exotic non-equilibrium condensed phases of hydrogen that could be useful for a wide range of energy applications.

Figure 1. Confinement of hydrogen in nanoporous materials can lead to manipulation of the hydrogen phase diagram, as shown by neutron scattering studies under a range of pressures and temperatures \cite{2}

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  \item \cite{2} Terry, L. R., Rolls, S., Tian, M., da Silva, I., Bending, S., Ting V.P., Manipulation of the crystalline phase diagram of hydrogen through nanoscale confinement effects in porous carbons, \textit{Nanoscale}, 2022, 14, 7250-7261
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