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The State and Phase of Nanoconfined H₂

Neutron diffraction and spectroscopy study of H₂ adsorbed in micro and mesoporous activated carbons

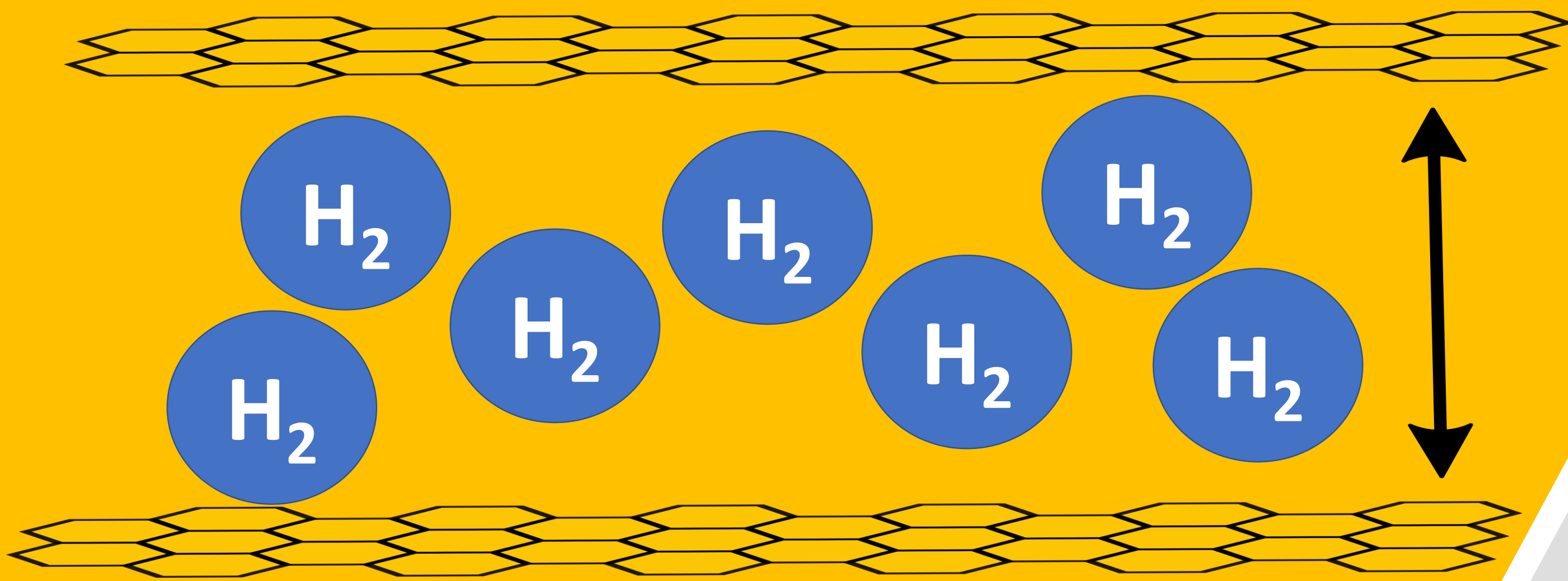
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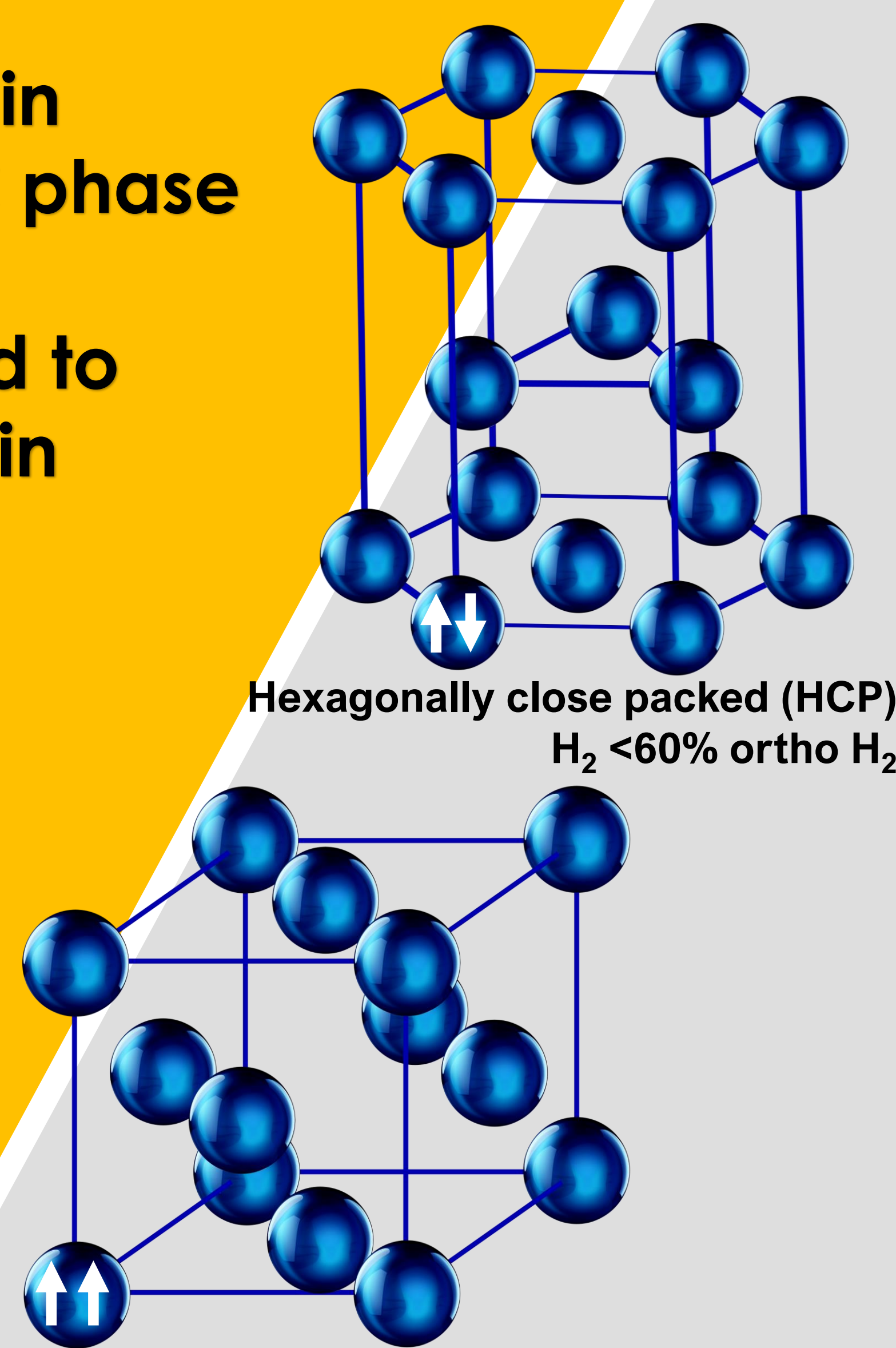


Summary

Crystalline H₂ observed in activated carbons. FCC phase observed at elevated temperatures compared to bulk and in higher ratio in microporous carbon

Conclusion

Nanoconfinement increases thermodynamic stability of FCC solid phase due to carbon - ortho H₂ interaction

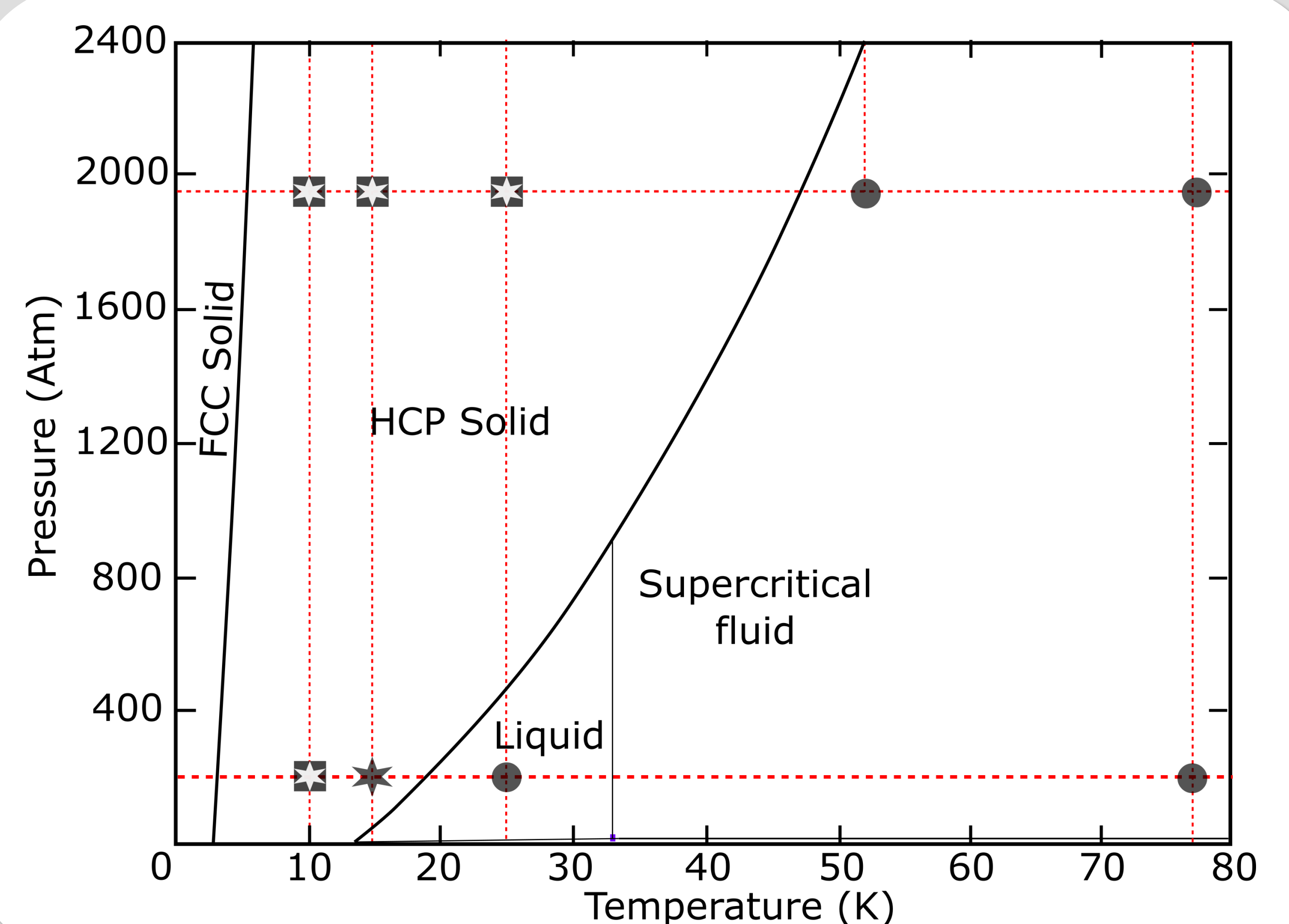


Background

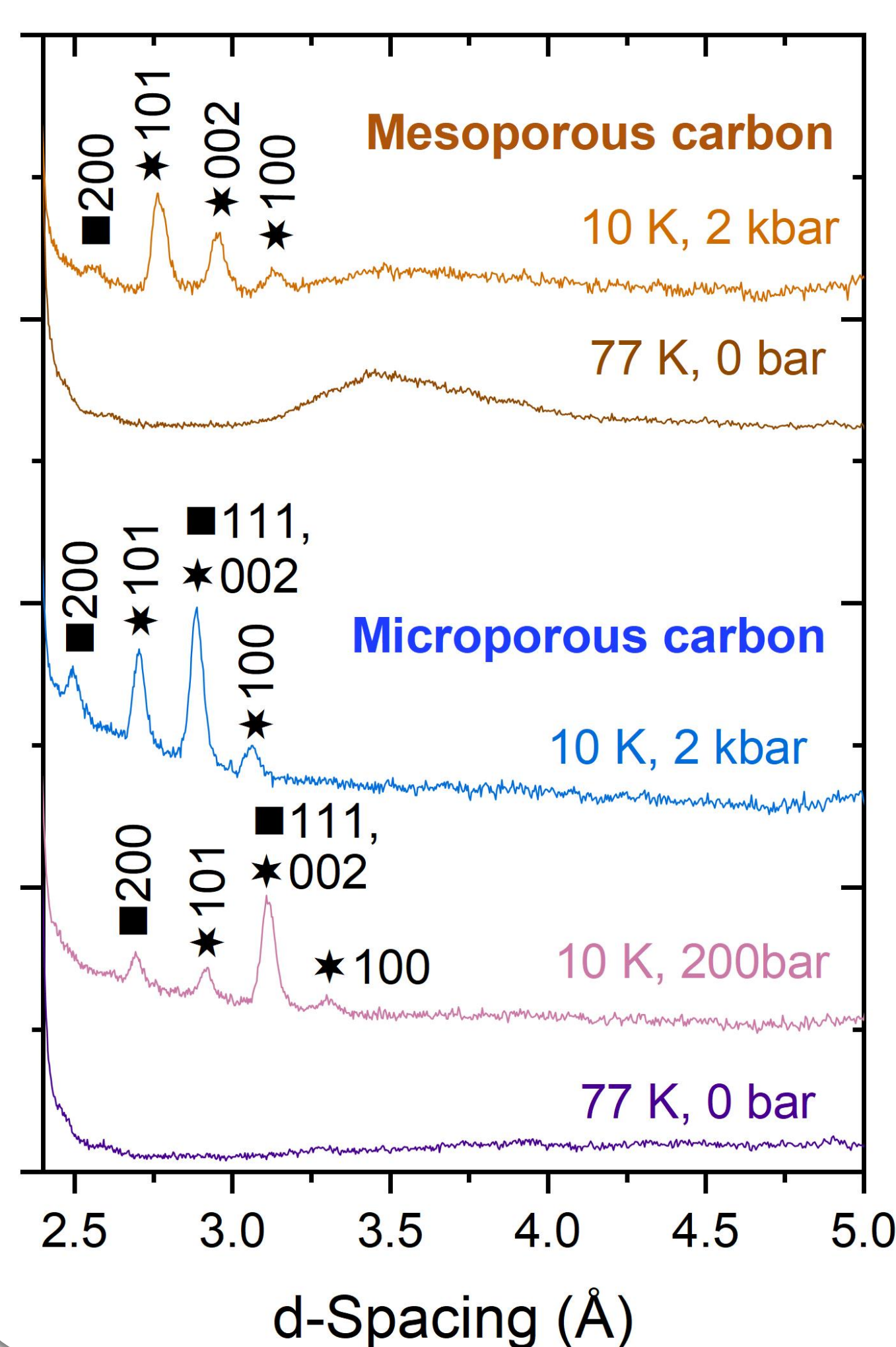
At low pressures and temperatures, two crystalline phases of H₂ are known: hexagonally close packed (HCP) and face-centred-cubic (FCC) H₂. FCC forms only when ortho concentration is >60 %. Recently it has been demonstrated that H₂ adsorbed into highly microporous carbon (< 2nm) becomes immobile and reaches densities above that of bulk liquid and solid above the critical temperature [1,2,3]. If this is true, then understanding the mechanism as to why and how these dense phases form would be vital to enhancing the storage capacity of these materials.

Aim

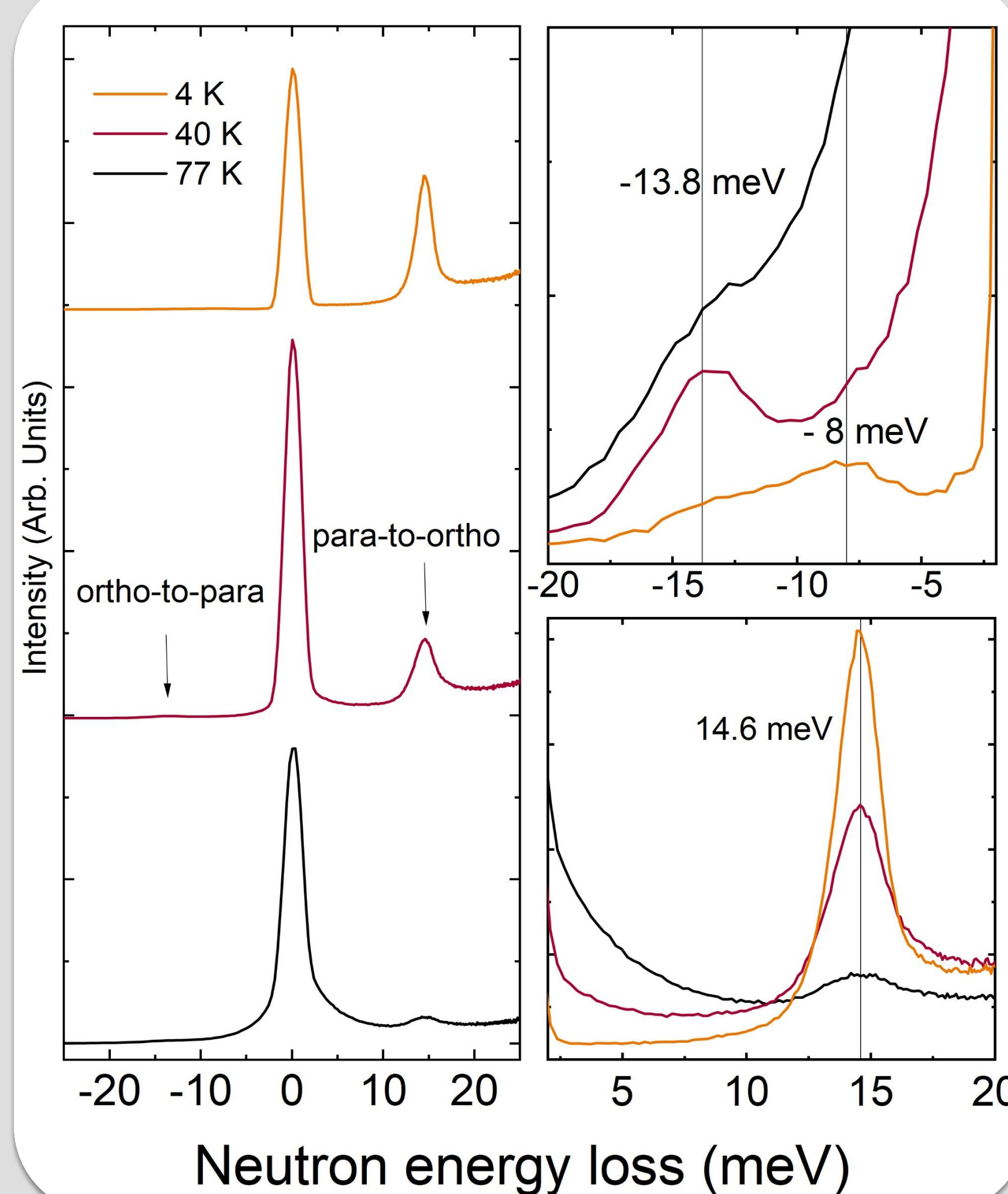
Determine the state & phase of H₂ confined in the pores of mesoporous (2-50 nm) Vs. microporous (< 2nm) activated carbons at temperatures across the bulk solid & liquid phase boundaries



Confined FCC H₂ observed at temperatures above the bulk: Bulk phase diagram of pure ortho H₂ overlaid with microporous carbon + H₂ neutron diffraction results. Red lines represent the experimental pressures and temperatures, squares represent FCC phase, stars represent HCP phase and filled circles short-range-order.



Increased FCC H₂ observed in microporous carbon: Neutron diffraction of microporous TE7 and mesoporous OLC porous carbons shows increased fraction of FCC phase (squares) over HCP phase (Stars) in microporous carbon.



Carbon - ortho-H₂ interaction: Temperature-dependent inelastic neutron scattering spectra of microporous carbon shows ortho-H₂ is rotationally hindered, whereas para-H₂ freely rotates, meaning ortho-H₂ is more strongly bound to the carbon.

Results

- Phase I HCP and FCC H₂ observed in both meso and microporous carbon.
- Microporous: up to 4.7 times more FCC to HCP
- Mesoporous: up to 0.3 times less FCC to HCP
- Confined FCC phase observed above bulk transition temperature
- Confined HCP obeys bulk transitions
- Confined H₂ unit cells are larger than bulk H₂
- Short-range-order observed in the bulk fluid range
- Inelastic neutron scattering reveals confined ortho-H₂ is more strongly bound in carbon compared to para-H₂**

Methods and Materials

- Neutron Diffraction - GEM, ISIS - UK
- Inelastic Neutron Scattering - IN4, ILL - France
- Mesoporous OLC (modal pore width 9.9 nm)
- Microporous TE7 (modal pore width 0.55 nm)
- Degas, 350 C, 1x10⁻⁶ mbar, +8 hrs
- 99.999% n H₂

[1] Ting et al, ACS Nano, 9 (2015)
[2] Gallego et al, JACS, 133 (2011)
[3] Olsen et al, ACS Nano, 11 (2017)

