Gas Adsorption in Metal Organic Frameworks

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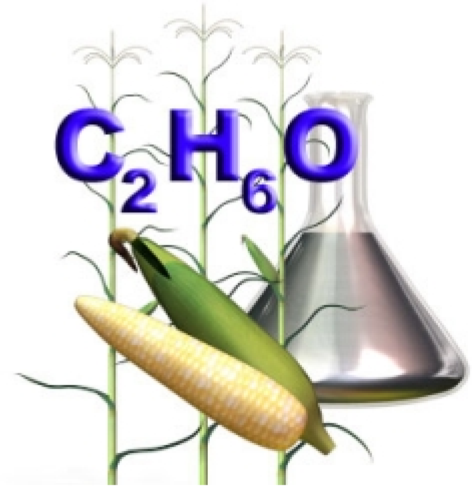
Overview

- Challenges facing energy storage
- Applications of neutron scattering
  - Locations of molecules
  - interaction strengths
- Future directions
- Conclusion

Transportation fuels (away from gasoline)



Congress initiative

$1.2 Billion to develop the technology for commercially viable hydrogen-powered fuel cells (2003)

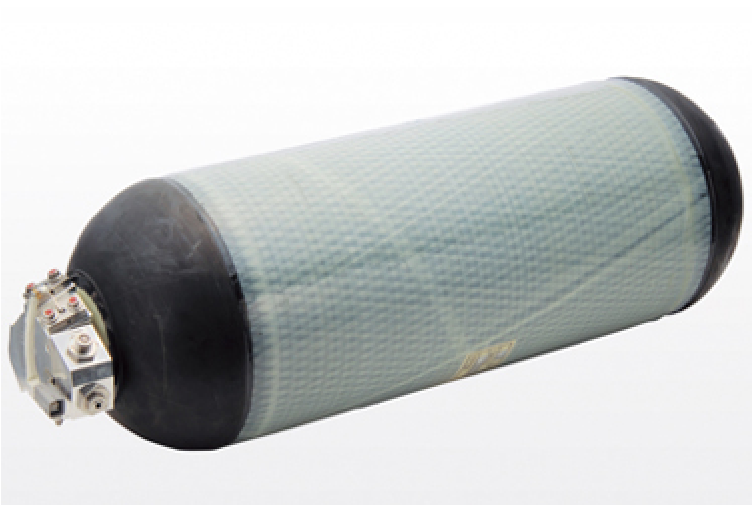
Why hydrogen is special

H_2 has 3x energy content by mass c.f. gasoline

Gasoline has 4x energy content by volume c.f. H_2

Schlapbach and Zuttel (2001) *Nature* 414: 353-358

Challenges



- Weight and volume
- Efficiency
- Refueling time

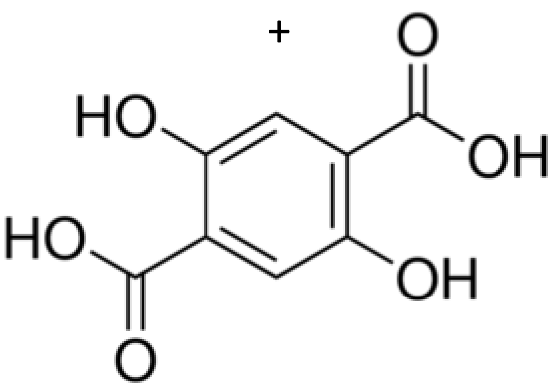
DoE 2020 Storage Targets

Gravimetric capacity	5.5 mass% H_2
Volumetric capacity	40 g H_2/L
Operating temperature	-40 to 60 °C
Maximum pressure	100 bar
Refueling rate	1.67 kg H_2/min
Cost	$333 per kg H_2

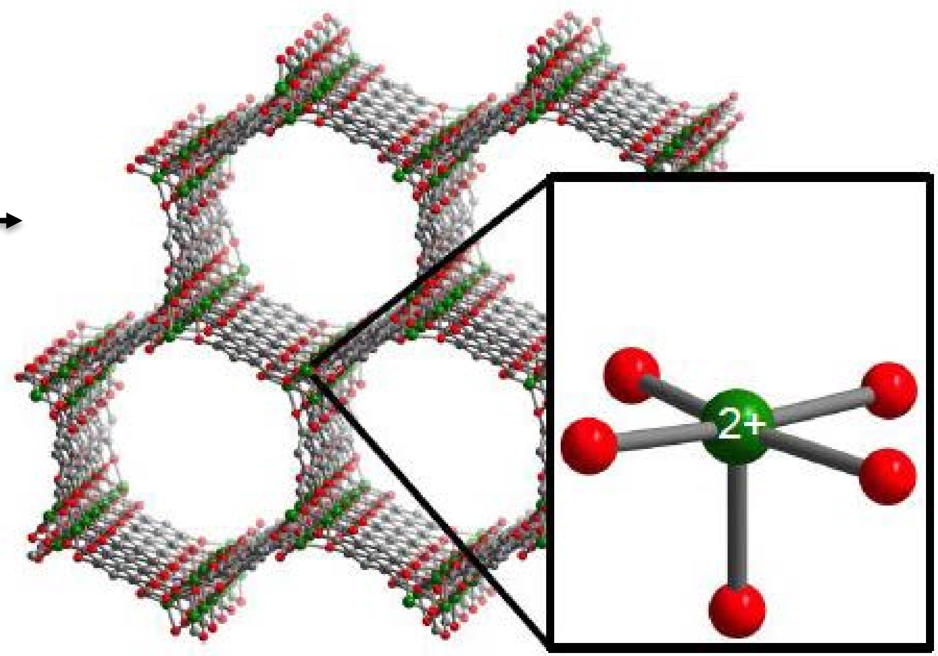
A Metal Organic Framework (MOF) with a high density of exposed M^{2+} sites

$MX_2 \cdot 6H2O$

+



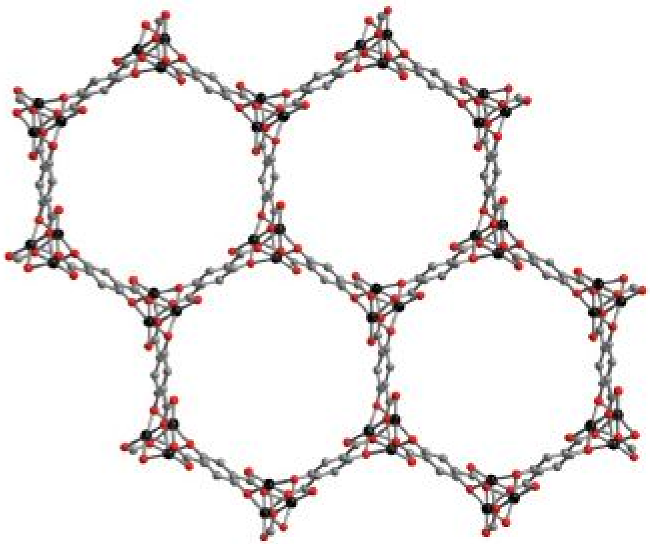
H_4dobdc

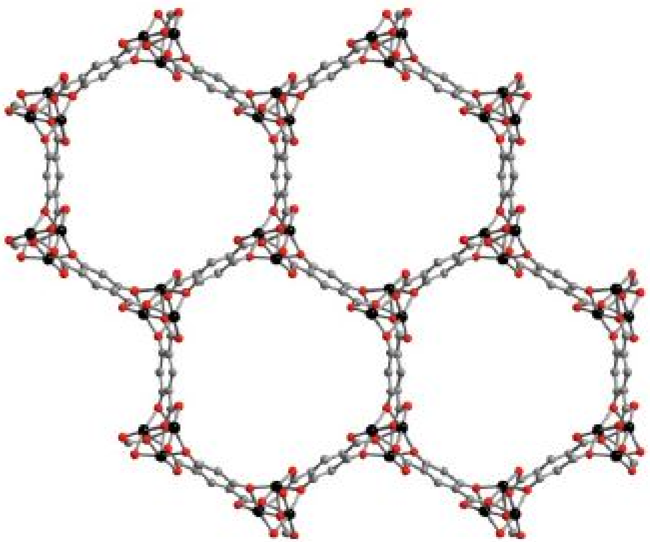


M_2 (dobdc), M-MOF74

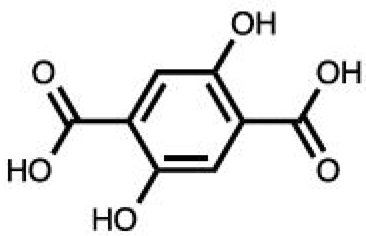
M= Mg, Mn, Fe, Co, Ni, Cu, Zn

Co_2(*m*-dobdc)

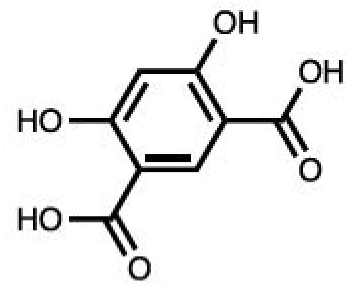




H_4(dobdc)

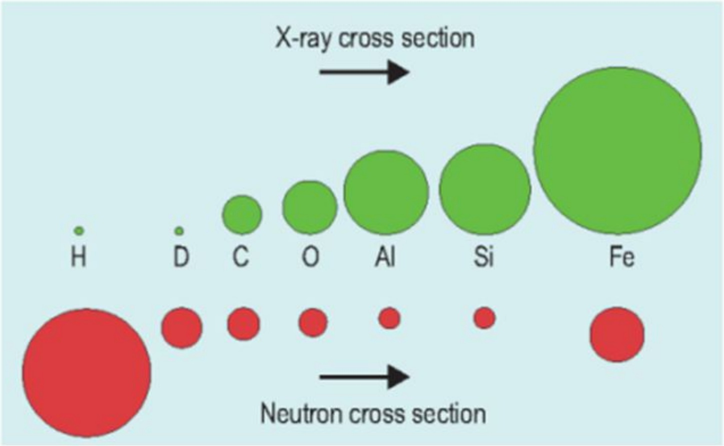


H_4(*m*-dobdc)

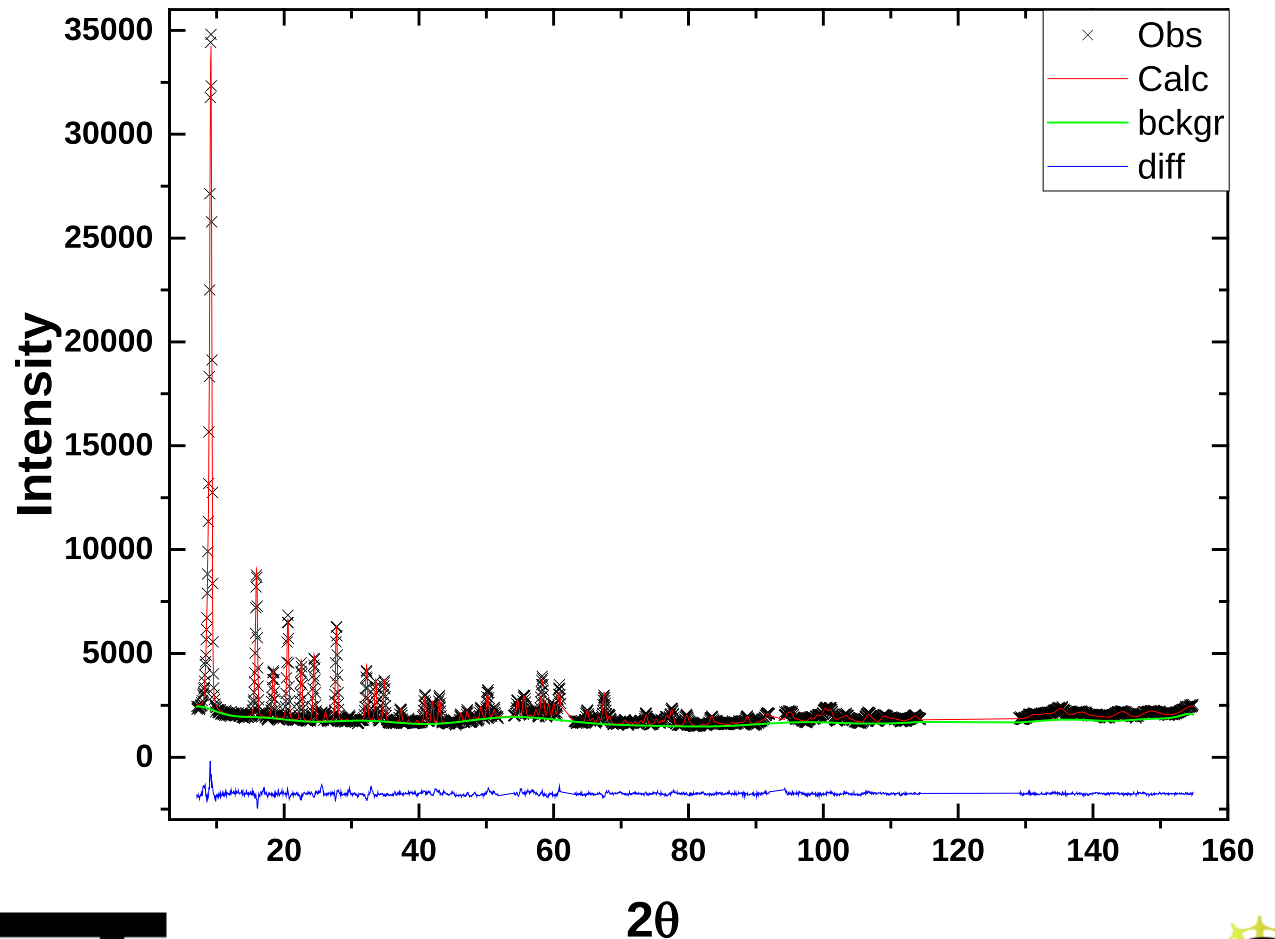


How and Why

Comparison of Neutron and X-ray cross sections

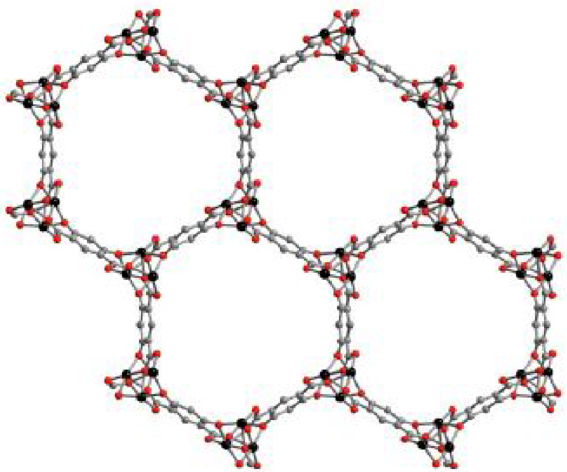


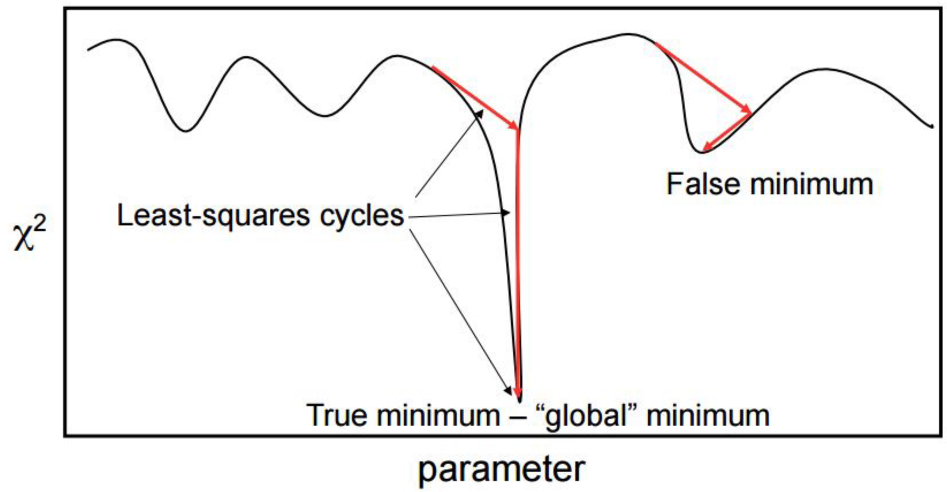
Where are the deuteriums-Bare $Co_2(m\text{-dobdc})$



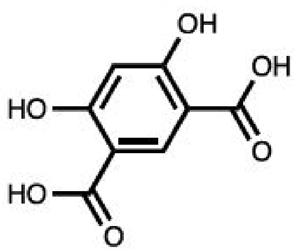
χ^2=1.928

Refinements in GSAS

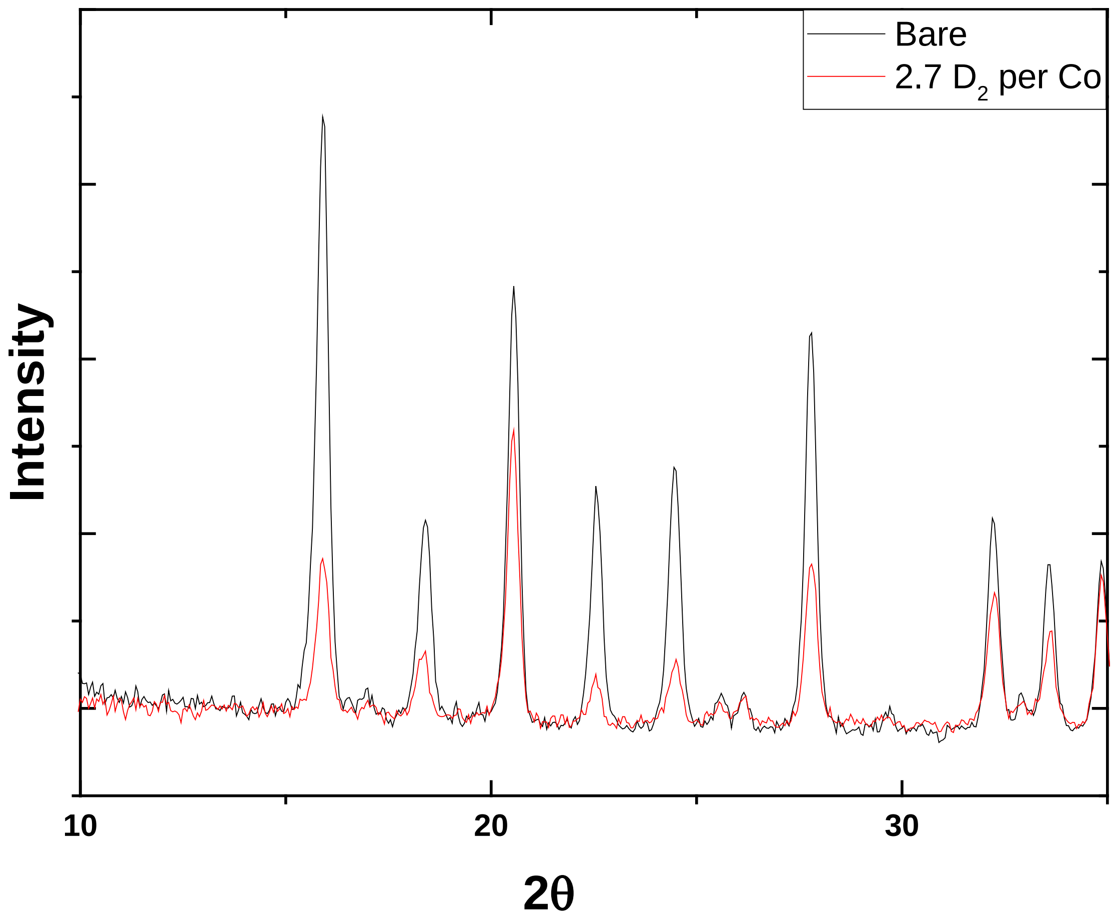




H_4(*m*-dobdc)



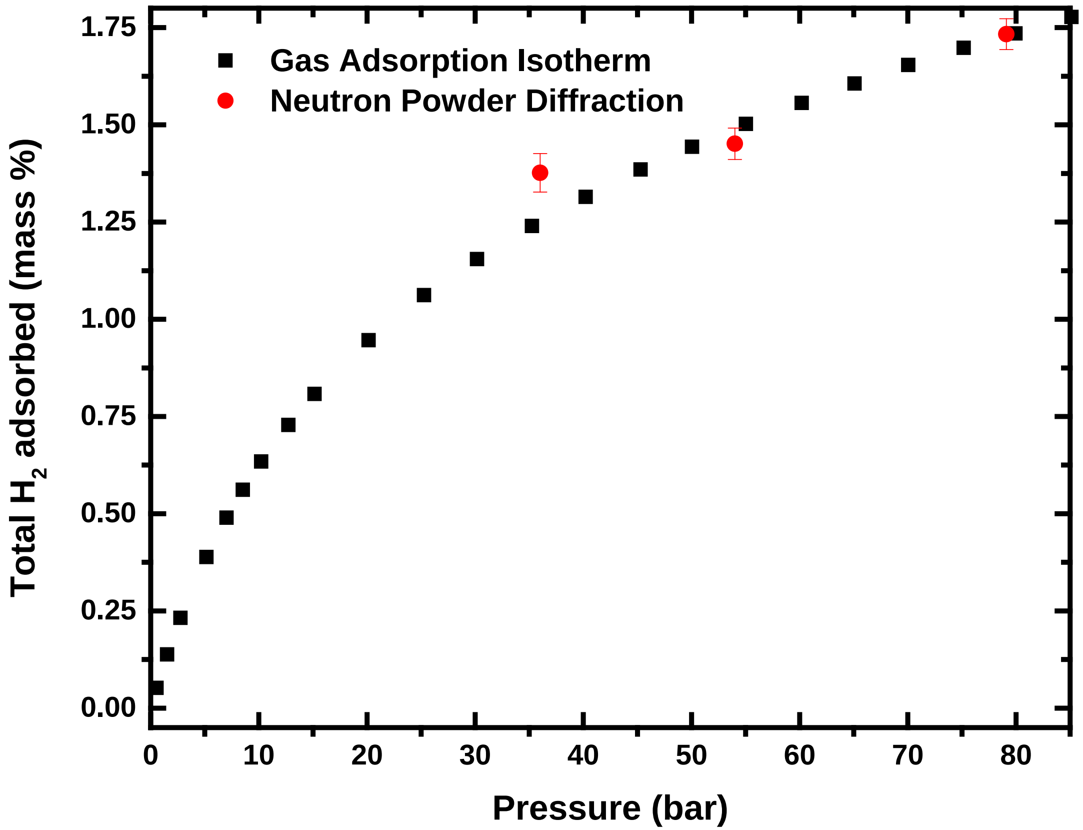
Where are the deuteriums?



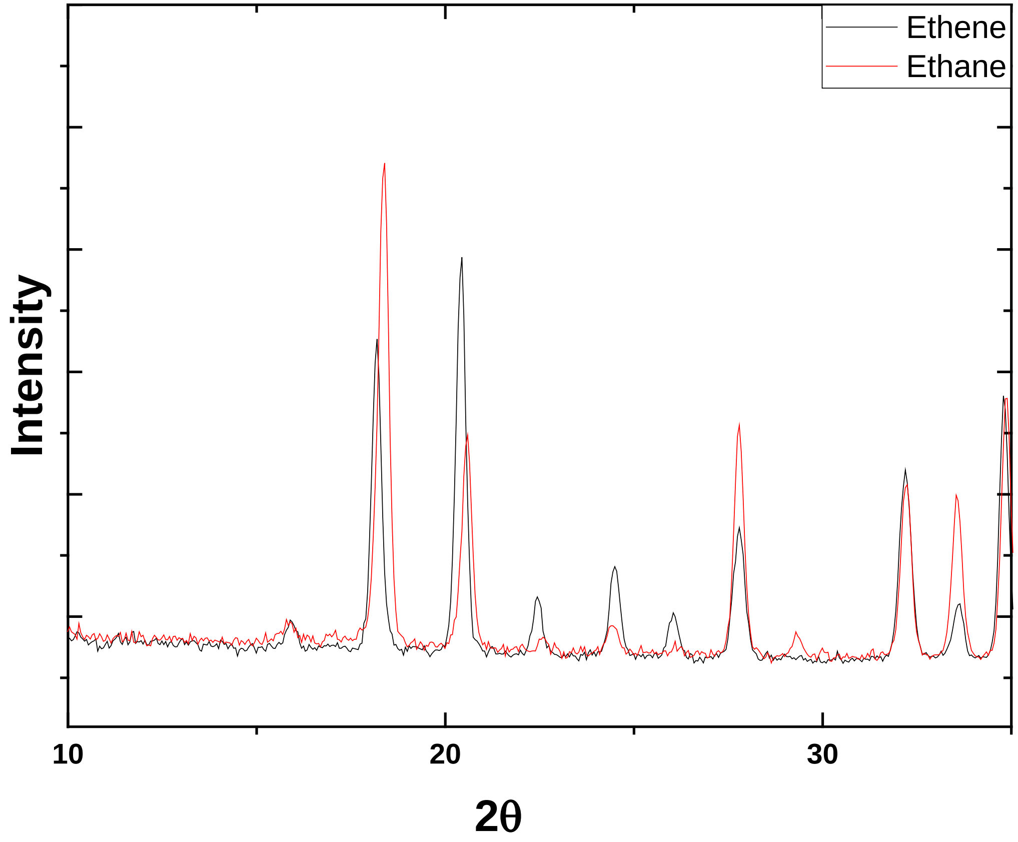
Where are the deuteriums?

Fourier difference to locate D_2 in Co_2 (*m*-dobdc)

Gas adsorption isotherms



Future directions-Hydrocarbon separations



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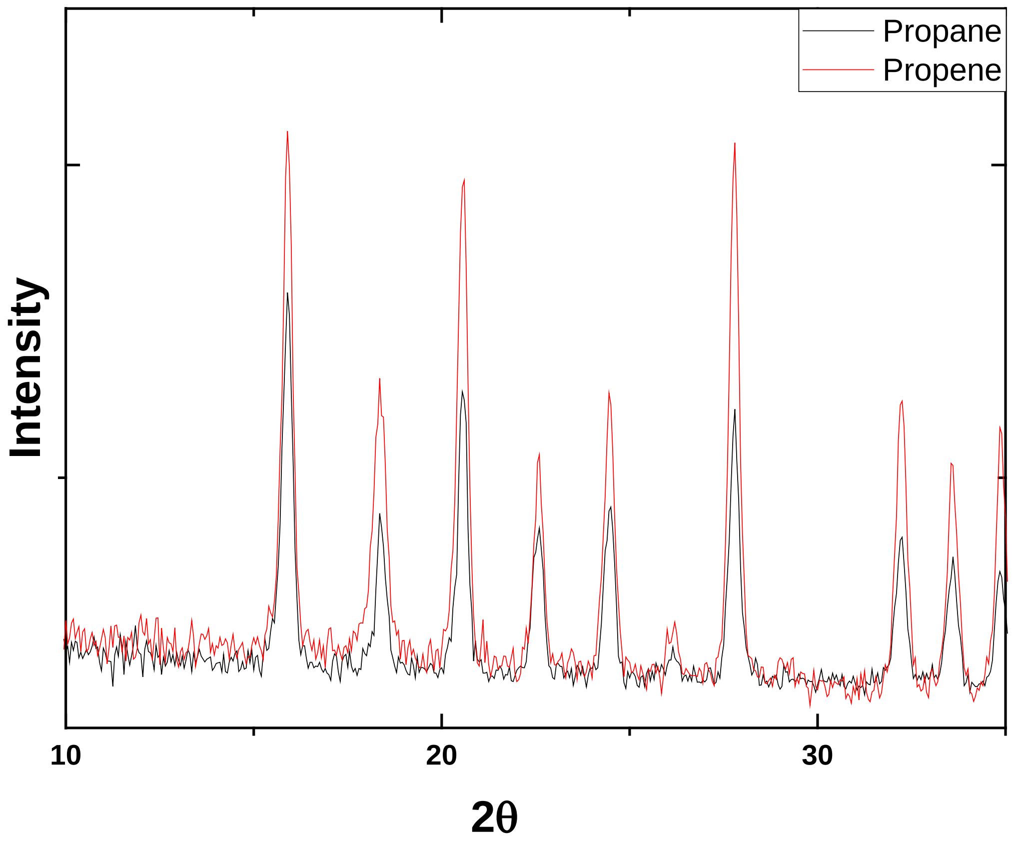

Conclusions

- Neutrons used to validate storage capacity
  - Reveal location of gas at angstrom scale
- Diffraction shows clear differences in affinities for small hydrocarbons
  - Refinements coming soon

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