Contribution ID: **32** Type: **Invited**

Investigating guest selectivity and dynamics in porous framework materials using in situ neutron scattering and computational approaches

Wednesday 20 July 2016 11:50 (20 minutes)

Microporous solids capable of reversibly hosting specific guest molecules are being actively sought for a wide variety of applications in the energy sector, including CO_2 sequestration and conversion, gas separations, fuel storage, and catalysis. Classes of porous framework materials such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) are considered especially promising for such applications due to their unrivalled structural and chemical tunability with respect to traditional solid sorbents such as zeolites [1].

Rational tuning of a framework material for improved performance requires that the nature of the interactions between the host framework and guest molecules be well-understood at the atomic level. Our research targets this detailed understanding of framework-guest systems using in situ neutron scattering experiments in which the framework structure and dynamics are probed as a function of guest loading and temperature. Rapid measurements performed using the high-intensity neutron diffractometer WOMBAT at OPAL (Australia) can capture structural changes in the framework before equilibration with the adsorbate, allowing us to approach more closely the real-world behaviour of a sorbent operating under continuous flow conditions. Our experimental results are supported by comprehensive atomistic density functional theory-based (DFT) calculations from which various physical and dynamical properties are extracted.

We are currently investigating several MOFs which display unexpected sorption properties such as "reverse sieving"–that is, selectively absorbing larger gas molecules while rejecting smaller ones. Using in situ neutron diffraction to locate the preferred binding sites of guest molecules in the framework, inelastic neutron scattering methods to probe guest-dependent lattice dynamics and guest diffusion characteristics, and DFT molecular dynamics simulations to validate and interpret our experimental results, we are able to gain detailed information about the mechanisms of gas uptake and selectivity in these exciting new MOF materials.

[1] Li JR, Kuppler RJ and Zhou HC (2009) "Selective gas adsorption and separation in metal-organic frameworks", Chemical Society Reviews, 38:1477-1504.

Author: AUCKETT, Josie (The Bragg Institute, Australian Nuclear Science and Technology Organisation)

Co-authors: DUYKER, Samuel (School of Chemistry, The University of Sydney); PETERSON, Vanessa (The Bragg Institute, Australian Nuclear Science and Technology Organisation)

Presenter: AUCKETT, Josie (The Bragg Institute, Australian Nuclear Science and Technology Organisation)

Session Classification: Session VII: Catalysis (Chair Mikhail Feygenson)