Oral Contributions

[MS27 - 02] In situ crystallographic studies of adsorption processes in functional porous materials. Phoebe K. Allan[a], Karena W. Chapman[b], Catherine L. Renouf[c], Peter J. Chupas[b], Simon J. Teat[d], Elizabeth K. Howe[a], Joseph A. Hriljac[e], Clare P. Grey[a], Russell E. Morris[c]

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Porous materials find potential application in a wide range of technologies including gas storage and separation and electrochemical devices [1,2]. Characterisation of these materials in 'real-life' operating conditions using *in situ* experiments can give unparalleled information aiding the elucidation of links between the structure of the materials and the observed physical properties. However, many interesting materials lack long-range order during some or all of their function, making characterisation using Bragg methods challenging. This can be further complicated by adsorption of ions or gas molecules in the pores of the materials. This talk will focus on *in situ* total scattering methods, which utilize, but do not rely on any Bragg scattering from a material, and their use in combination with other crystallographic and spectroscopic techniques to determine structural information about adsorbents in porous materials. First, work using Bragg and total scattering techniques to determine the structure of molecules of medical gases nitric oxide and hydrogen sulfide within metal-organic framework materials will be presented [3]. *In situ* single-crystal methods using a specially designed environmental gas cell are used to characterise the uptake and release of nitric oxide gas from the metal-organic framework Co-CPO¬27; the crystallographic results correlating well with gas adsorption isotherms [4]. These single-crystal methods are extended and combined with complementary pair distribution function (PDF) analysis to analyse a thermally activated single-crystal to single-crystal structural transition in framework Cu-SIP-3, and to probe the material's ultraselective adsorption for nitric oxide [5]. The structure of the Ni-CPO-27 hydrogen sulfide-adduct determined by both powder X-ray diffraction and differential pair distribution function methods reveal the open-metal site as the primary adsorption interaction in the material [6]. Next, the use of PDF analysis to determine the secondary building block of a new metal-organic framework and to verify the structural solution determined from powder X-ray diffraction data is presented. Finally, a discussion of more recent work combining PDF analysis and X-ray adsorption spectroscopy for the characterisation of electrolyte ions adsorbed in porous carbon electrodes for high power electrochemical applications will be presented.

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