Dr Valeska Ting's Abstract

Rapid and routine determination of hydrogen positions in inorganic and organometallic compounds

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Hydrogen is a fundamentally important element in many key areas of inorganic materials design, including development of technological materials (e.g. hydrogen storage media and proton-conductor fuel cell components), functional framework materials (e.g. zeolites), inorganic catalysts, organometallic coordination complexes and inorganic hydrates. Due to the weak scattering of X-rays by light elements, and hydrogen’s large incoherent neutron background, determination of hydrogen positions in inorganic materials, where possible, traditionally necessitates costly sample deuteration or painstaking synthesis of large single crystals for neutron diffraction. This limitation is now being addressed through the development of experimental and data refinement methodologies which utilise very high flux neutron powder diffractometers, such as D20 at ILL.

We will present a selection of crystallographic results demonstrating application of this new methodology to several technologically important inorganic material systems with significant hydrogen content. These include in-situ studies of functional zeolites containing adsorbed hydrogenous molecular species and metal ammoniates such as Ni(NH3)6Cl2 (candidate hydrogen storage materials). Further examples will include organometallic compounds such as Zeise’s salt and complexes where exact determination of hydrogen position, e.g. those with potential agostic hydrogens, is needed. The full structures of a series of heavy metal salt hydrates will also be presents, confirming that hydrogen positions can be accurately determined in the presence of metals as heavy as uranium and bismuth.

As well as highlighting the applicability and potential impact of these new methods, this work is aimed at establishing these methodologies as a valuable tool for the routine study of hydrogenous materials across all inorganic fields.

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