Science and Technology Facilities Council

Demonstrating the viability of a scalable route to synthesise a gas storage material

Sustainable technologies company, Johnson Matthey, used neutron scattering to track the synthesis of a commercially relevant porous material, suitable for gas storage and catalysis. The results provided insights to develop a more economic, sustainable and scalable production pathway.

Challenge

Zeolitic imidazolate frameworks (ZIFs) are porous materials with many potential applications, including gas separation, catalysis, electronic devices and drug delivery. For ZIFs to be used industrially, large-scale production routes are needed. Where conventional, small-scale syntheses often use large quantities of expensive and toxic solvents, such as methanol, large-scale production requires economic and environmentally friendly alternatives.

Researchers from Johnson Matthey wanted to investigate the feasibility of preparing ZIF-8 by first synthesising a different material, ZIF-L, and then transforming this into ZIF-8, as this novel route uses much less water and organic solvent.

Solution

The team from Johnson Matthey used several techniques, including neutron scattering at ISIS Neutron and Muon Source, to track the transformation of ZIF-L into ZIF-8 and demonstrate a scalable route to synthesise ZIF-8.

Benefits

By using neutron spectroscopy, Johnson Matthey gained better understanding of the chemistry of their production process and showed that the synthesis of ZIF-8 was successful. The study also demonstrated that neutron spectroscopy could be used to track the reaction in real time, which would be beneficial in material scale-up to determine when the transformation of ZIF-L to ZIF-8 is complete.

On scaling production, Johnson Matthey successfully synthesised one kilogram of ZIF-8, with the potential to increase industrial production to 15 tonnes per year. The pilot formed the basis of an economic analysis that showed this synthesis route could produce over six times more ZIF-8 than direct methods. The results will aid Johnson Matthey in developing larger-scale processes that produce more material at a lower cost, whilst also reducing environmental and safety concerns.

> **“INS spectroscopy conducted on the TOSCA beamline at ISIS allowed scientists at Johnson Matthey to probe the structure of ZIF-8 and its polymorph ZIF-L. Data collected on TOSCA gave our scientists high confidence when working towards an accurate and predictive cost model with the ultimate aim of Metal-organic Framework commercialisation.”**
>
> Timothy Johnson, Senior Scientist, Johnson Matthey

ISIS Neutron and Muon Source

ISIS Neutron and Muon Source has successful collaborations with many different industries, delivering insights to develop new and improved materials and processes.

Why use neutrons?

Study structure
Neutron wavelengths are comparable to the spacings of atoms and molecules.

Study dynamics
Neutron energies are comparable to the time scales of molecular diffusion, vibrations and rotations.

Study magnetism
The neutron's magnetic moment can be used to study the microscopic magnetic properties of materials.

Penetration power
Neutrons can penetrate deep into matter (including many different metals) enabling the study of large samples – even within complex sample environments.

Non-destructive
As a non-destructive, non-invasive probe, neutrons are suitable for the characterisation of delicate and precious samples.

Versatile sample environments
Sophisticated sample environments enable measurements under operating conditions – including extreme temperatures and pressures.

Sensitivity to light elements
The neutron scattering power of nuclei varies in a random manner such that lighter atoms (e.g. H, Li) can be studied in the presence of heavier ones.

Isotopic contrast
Neutrons are sensitive to different isotopes of the same element, so isotopic substitution (e.g. H/D) can be used to highlight specific structural features.

Complementarity
Neutron scattering is highly complementary to other techniques, such as X-ray scattering, electron microscopy, magnetic resonance and computational methods.

How to work with ISIS
ISIS offers industrial users access to advanced analytical techniques and expert scientific and technical support for materials characterisation. Access options include proprietary use, academic partnerships, grant funded access, and the Industrial Collaborative Research and Development (ICRD) program.

For more information, email ISISindustry@stfc.ac.uk to discuss the most suitable method to solve your challenge.