Laidlaw Research Proposal: Tailoring the Flexible Zeolite Molecular Sieve Merlinoite for Carbon Capture

Aim

To synthesise various lithium-exchanged merlinoites with high silicon/aluminium ratios. To characterise the adsorption behaviour of these materials, using adsorption isotherms, and considering hysteresis effects. To develop an analytical model for the adsorption of gases, in particular carbon dioxide, for merlinoites which can account for the impact of dynamic structure changes and gating effects on the kinetics of adsorption. To refine models for the structure of the synthesised materials using Rietveld analysis.

Planned Synthesis

The synthesis will be an interzeolite conversion using a precursor, zeolite Na-Y or an ion-exchanged derivative. Initially, a strongly basic solution is made up, to which a silica suspension is added as a source of silicon to increase the Si/Al ratio of the product zeolite. To this the precursor zeolite is added, forming a colloidal suspension. This is thoroughly mixed and heated for around three days with continuous tumbling to produce a homogenous sample of the desired merlinoite.

Planned Analysis

The solid product will be analysed using powder X-ray diffraction (PXRD). Potentially silicon-29 nuclear magnetic resonance spectroscopy (^{29}Si-NMR) and aluminium-27 nuclear magnetic resonance spectroscopy (^{27}Al-NMR) will be used in addition, to confirm purity and to provide further information. The data acquired will be used for structure refinement by Rietveld analysis.

The gas adsorption behaviour of the synthesised materials will be analysed under isothermal conditions to elucidate the uptake capacity and its response to structure changes. The kinetics of the adsorption will also be investigated and compared to the developed analytical model(s).

Potential Conclusions, Motivation and Background[1]

The conclusions will hopefully inform further research and industry use of merlinoites for a variety of applications utilising selective adsorption of carbon dioxide, for example in carbon capture, gas separation in industry, and natural gas upgrading.

Current techniques for these processes, mostly based on cryogenic gas separation, have significant environmental and financial costs due to high energy and time demands. Zeolite-based separation technologies can have significantly lower negative impacts as they require substantially less energy, minimal additional processing, and utilise reusable, cheap and extremely safe materials.

Wide-spread adoption of zeolite-based adsorption technologies for carbon capture could contribute to a dramatic reduction in the estimated 10-15% of global energy consumption that gas separation is responsible for.

[1] **Relevant recent review:** Bai, Ruobing, Xiaowei Song, Wenfu Yan, and Jihong Yu. 2022. "Low-Energy Adsorptive Separation By Zeolites". *National Science Review* 9. doi:10.1093/nsr/nwac064.