A computational screening of porous materials for biogas upgrading

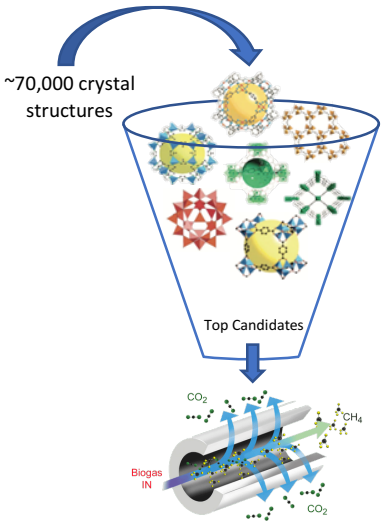
Elena Besley, Joseph Glover, Aidan Manley

School of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

Biomethane derived from biogas can be used as source for energy storage and transport applications. Mainly composed of CH_4 (50-70%), biogas also contains large quantities of CO_2 (35-50%) and small amounts of various trace gases such as H_2S, N_2, H_2 and NH_3. Therefore, it is essential to employ purification methods to remove unwanted impurities and increase the calorific content of the gas. While conventional methods (ads/absorption, cryogenic sieving etc.) are highly effective at producing biomethane content with greater than 95% purity, they suffer from high investment and operational costs. In recent years, membrane technology has received much attention due its promise as a cheaper alternative.

The use of mixed matrix membranes (MMM), made from organic polymers and porous filler particles, combines the exceptional mechanical properties of pure organic membranes and high selectivity, permeability and tuneability provided from inorganic membranes, into one hybrid. Typical porous filler particles include carbon-based materials, zeolites, metal-organic frameworks (MOFs), covalent-organic frameworks (COFs) and more. However, with such breadth of choice, one of the main challenges of designing new MMMs is knowing which filler particles will provide high permselectivity and be compatible with the organic polymer.

In these situations, the use of high-throughput computational modelling can be an effective and rational means of identifying real and hypothetical candidates for separation and storage applications. In this work, a multi-level screening protocol combing various classical simulation techniques is used to screen approximately 70,000 MOFs and COFs as MMM filler particles for biogas upgrading. Initial candidates are quickly screened based on their permeabilities at infinite dilution, to assess the interaction strength between guests and the frameworks. Strong candidates are then subject to more accurate grand-canonical Monte-Carlo and equilibrium molecular dynamics simulations at working conditions of 10 bar and 298 K.



Screening candidates for biogas separation

This approach aims to develop a better understanding of the structure-performance relationships that govern CH_4 separation from biogas with the hope of aiding both computational and experimental design of novel membranes. In addition, we are able to identify promising experimental crystal structures that may not have been previously considered for separation applications.