Proposal ~500 words

This project plans to run a computational screening of metal organic frameworks (MOFs) from the Cambridge Structural Database (CSD) to search for suitable structures for the selective adsorption of helium gas over the main components of natural gas reserves, nitrogen and methane.1 Several layers of calculations will be run to reduce the initial ~100000 structures down to ~100 for closer analysis. Characteristics of the final set will be investigated to determine the features of a MOF that may indicate good preferential helium separation.

MOFs that cannot physically adsorb Helium will be initially screened out by calculating pore window sizes and volumes, and other confounding factors such as solvent molecules occupying pores in the crystal structures. These calculations will be performed through python scripts that access the CSD for MOF structures.

Grand Canonical Monte Carlo simulations2 will be performed through RASPA2 to determine the Henry’s constant for helium, nitrogen and methane adsorption into each MOF that passes through the first phase/s of calculations. These will/may also be performed to determine constants for other noble gases or gases present in natural helium-containing deposits such as ethane and water.

All calculations will be run from the Eddie supercomputer3 due to the strenuous computational requirements for processing a dataset as large as the Cambridge Structural Database. Results will be compared with the 2019 paper from Zabradi-Poor and Marek4 using similar methods on a smaller dataset to both check for concordance and potentially to find helium adsorbing MOF structures that were not previously characterised.

Results from calculations will also be compared to literature experimental results, when possible, through use of the NIST database of novel and emerging adsorbent materials (DNEM)5. This database contains isotherms and information on the adsorbent properties of a range of MOFs, and can provide empirical backing to support any observations made from our simulations.

Additionally, MOF properties relevant to their thermal stability will be investigated to identify potential problems with industrial use of the most highly helium selective MOFs. Factors that may cause a MOF to break down or otherwise not function in the conditions required for bulk helium production will be identified and from this, a final check can be performed on the MOFs from calculation to determine their viability in replacing existing helium producing systems. The environmental cost to the production of high selectivity MOFs will also be investigated against current helium production to further prove or disprove their potential viability.

References

1. <https://journals.sagepub.com/doi/epdf/10.1260/0263-6174.32.1.49>
2. <https://www.tandfonline.com/doi/abs/10.1080/00268977500100221>
3. https://www.ed.ac.uk/information-services/research-support/research-computing/ecdf/high-performance-computing
4. <https://pubs.acs.org/doi/10.1021/acs.jpcc.8b07804>
5. https://adsorption.nist.gov/isodb/index.php#home