Proposal ~500 words

This project plans to run a computational screening of MOFs from the CCDC 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. A parallel screening will be run to determine if similar MOF properties are relevant to the selective separation of larger noble gases from both nitrogen and the other group 8 elements.

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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 Cambridge Structural Database for MOF structures.

Grand Canonical Monte Carlo simulations 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 supercomputer due to the strenuous computational requirements for processing a dataset as large as the Cambridge Structural Database. Results will be measured against the 2019 paper using a similar method2 on a smaller dataset to both check for concordance and potentially to find helium adsorbing MOF structures that were not previously discovered.

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Additionally, MOF properties relevant to their thermal stability will be investigated to determine potential problems with use of highly helium selective MOFs. Factors that may cause a MOF to break down or otherwise not function in the conditions required for industrial 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 their potential viability.

References

1. <https://journals.sagepub.com/doi/epdf/10.1260/0263-6174.32.1.49>
2. https://pubs.acs.org/doi/10.1021/acs.jpcc.8b07804