Resources required:

The Eddie supercomputer HPC (High performance computing) facilities will be used to perform grand canonical Monte Carlo (GCMC) simulations, implemented in the RASPA suite of codes. They will be used to compute adsorption isotherms of various gases in different MOFs. The Cambridge Structural Database (CSD) will provide the dataset of the MOFs studied (over 100,000 MOFs). They will allow to study several API (Absorbance Performance indicator) of MOFs, such as pore volumes, densities, surface areas, limiting pore diameters (LPDs) and largest cavity diameters (LCDs). The NIST website provides data on different adsorbent/adsorbate isotherms. Henry’s constants will be computed using the Widom insertion method in RASPA.

Cost per core hour: £0.02

The Eddie supercomputer has 7,000 cores but only one will be used.

Assuming an estimated time of a week processing time (50 hours), approximate cost would be: £1.00

The data costs £175.00 per TB. It is estimated that 50GB will be used. This will amount to roughly £8.75 spent on storage.