Resources required:

Linux and the 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.

It is estimated that …. will be spent on the HPC, approximating cost: …