Master Project

Supervisors

Prof. Berend Smit, berend.smit@epfl.ch

Dr. Fatmah Ebrahim, fatmah.ebrahim@epfl.ch

Raluca-Ana Kessler, raluca-ana.kessler@epfl.ch

Laboratory

Laboratory of Molecular Simulation (LSMO)

Contact

For more information regarding the project or for any other question, please contact Raluca Kessler (raluca-ana.kessler@epfl.ch)

Project Description

Metal-organic frameworks (MOFs) are promising solid sorbents. They comprise metal cations as nodes and functionalized organic ligands as linkers, that combine to form extended, crystalline, porous networks. This class of materials has attracted significant attention thanks to the possibility of targeting desired properties by altering the building units to make them suitable for many applications. MOFs offer an advantage in DAC by capturing CO2 through physisorption, chemisorption, or a mix of both, leading to lower regeneration temperatures than other sorbents. Despite research and databases with numerous MOFs, finding a suitable MOF for DAC remains challenging due to the need for high CO2 uptake at low pressures, excellent stability, low toxicity and simple synthesis. Additionally, while MOFs offer easier regeneration, the two main methods, temperature swing adsorption (TSA) and pressure swing adsorption (PSA), still demand significant energy. One way to overcome the regeneration issue is to use micro/nanomaterials which can provide enough heat to regenerate the MOF.

In this project, the student will be responsible for synthesizing micro/nanomaterials, the metal-organic framework (MOF), and a composite made from these materials. While the synthesis of the MOF and micro/nanomaterials is already established, the primary focus will be on the composite's synthesis. The student will have the opportunity to investigate, such as: different synthesis for the composite, or the impact of the size of the micro/nanomaterials and the MOF, or the effect of altering the composition of the micro/nanomaterials (for example, changing the ligand). The resulting composites, as well as the MOF and micro/nanomaterials, will be characterized using techniques such as: Powder X-Ray Diffraction (PXRD), Thermogravimetric analysis (TGA), Scanning Electron Microscopy (SEM), and N2 and CO2 adsorption. The characterization will help assess the impact of the micro/nanomaterials on the MOF's adsorption capacity and the effects of the varied parameters.