
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)

Project Description

Rising CO₂ levels in the atmosphere contribute significantly to global warming. While pre- and post-combustion methods help reduce CO₂ emissions, additional strategies are needed to meet the requirements of the Paris Agreement. Direct Air Capture (DAC), a Negative Emission Technology (NET), facilitates the removal of existing atmospheric CO₂ and is essential for achieving long-term climate objectives. However, selectively capturing atmospheric CO₂ is a significant challenge, requiring advanced materials and processes.

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 combination of both, leading to lower regeneration temperatures than other sorbents. However, the two main regeneration methods, temperature swing adsorption (TSA) and pressure swing adsorption (PSA), still demand significant energy. One solution is to use Magnetic Induction Swing Adsorption (MISA) which aims to incorporate magnetic micro/nanoparticles (MNPs) that generate heat under alternating magnetic field.

In this project, the student will be responsible for the synthesis and detailed characterisation of magnetic micro/nanomaterials, MOF, and a composite made from these materials. As the synthesis of the MOF and micro/nanomaterials is already established, the primary focus will be on developing and optimising the composite. The student will have the opportunity to investigate: different synthesis for the composite, 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.

The expected outcome of the project is a set of well-characterized sorbent composites with performance insights suitable for publication in a peer-reviewed scientific journal.