Name of supervisors: Prof Petra Ágota Szilágyi, Dr Ken Luca Abel
Preferred background of candidates: Chemistry/Materials Science
Number of available projects: 1
Preferred project period: between mid-July and end of August 2025

Project rationale

Biogas, a complex gas mixture with high methane concentrations, is a renewable resource obtained through anaerobic digestion of biomass. Although it can be burnt to generate heat or electricity, this releases CO_2, and the various contaminants abundant in biogas cause it to be a rather low-grade fuel. Instead of an energetic use of particularly the methane component of biogas, the ABIME (Advanced biogas-to-methanol electrocatalysis) project aims for a chemical valorisation of biogas. By selectively converting the methane in it to methanol, a highly potent greenhouse gas is converted to provide a valuable platform chemical.

The direct conversion of methane to methanol (M2M) is considered one of the holy grails in catalysis and has been researched for decades. A recent push in this field was stimulated by the structural clarification of monooxygenase enzymes, which are capable of oxidising methane to methanol and contain iron or copper in their active sites. To replicate the activity of these enzymes is the aim of the CUBE-project at the catalysis section. The ABIME project, however, follows an electrochemical approach, in which the rate of oxidation can be finely controlled by the applied potential. The challenge in this project is thus to produce electrodes equipped with efficient catalysts to promote the selective oxidation. A seemingly trivial, but important requirement for these catalysts is that they need to be electrically conductive in order to allow the electrons to reach the reactant molecules. Within a variety of candidate materials, metal-organic frameworks (MOFs) with meaningful electrical conductivity have recently emerged for electrocatalytic applications [1-4]. As the first step towards electrochemical biogas oxidation, the aim of this summer project is to **synthesize and characterise metal-organic frameworks with electrical conductivity** based on tripodal triphenylene linkers.

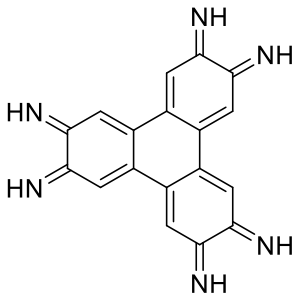


Figure 1 HITP (2,3,6,7,10,11-hexa-iminotriphenylene), a linker present in electrically conductive metal-organic frameworks [1,2,4].

Methodology

MOFs, built up of inorganic nodes interconnected by organic linkers in a regular and periodic fashion, typically exhibit high crystallinity and porosity. They usually contain pore channels, which not only provide a high surface area to enable chemical reactions, but also allows reactant molecules to pass through the material. Through the appropriate choice of the node and linker, networks with a variety of properties can be generated. In this project, we intend to use the HITP linker (Figure 1), which is available commercially, and combine them with divalent metal nodes (e.g., Mn, Co, Ni and Cu).

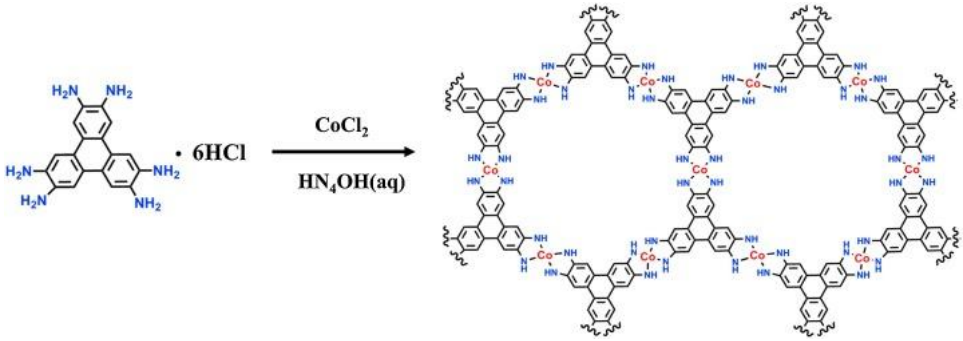


Figure 2 Proposed synthetic routes for $Co_3(HITP)_2$, one of the MOFs to be synthesized in the project [1].

The materials obtained will be characterised using powder X-ray diffraction to determine the crystal structure, N_2 sorption to study the porosity, Simultaneous Thermal Analysis (STA) to investigate the thermal stability, Nuclear Magnetic Resonance (NMR) Spectroscopy to analyse the ratio between linker molecules and capping agents and Scanning Electron Microscopy to study the surface morphology and elemental composition of the materials. If time allows for it, the preparation of electrodes from the synthesized metal-organic frameworks will be attempted.

Expected outcomes and deliverables

The expected project outcomes are as follows:

- Novel MOFs with redox activity and potentially electrical conductivity will be synthesized
- From extensive material characterisation, promising candidate materials for electrocatalytic testing will be identified
- The synthesis procedure of promising candidate materials will be optimized and potentially upscaled
- The student will receive cutting-edge training and valuable work experience.

The expected project deliverables are as follows:

- Novel MOFs with redox activity and potentially electrical conductivity, possibly also electrodes
- Project report
- Manuscript in Energy & Environmental Science / Advanced Materials, *etc.*

Project schedule

Week 1: H&S training, lab introduction/training; first MOF synthesis (small batch),
Week 2: MOF characterisation, first attempts to make analogues (small batch),
Week 3: MOF analogue characterization
Week 4: Optimisation/upscaling of synthesis for promising MOFs
Week 5: Characterisation of the MOFs from optimised/upscaled procedures
Week 6: Attempts to make electrodes from synthesised MOFs

References

[1] D. Sheberla *et al.*, *J. Am. Chem. Soc.*, 136, **2014**, 8859-8862.
[2] D. Xing *et al.*, *Appl. Catal. B.*, 278, **2020**, 119295.
[3] K-K. Liu *et al.*, *eScience*, 3, **2023**, 100133.
[4] M. McVea *et al.*, *Small Sci.*, **2025**, 2400469.