**Metal-Organic Frameworks (MOFs) as a disruptive solution for $CO_2$ capture in the presence of humidity** (in collaboration with Total-PERL)

Keywords: $CO_2$ – CCUS – MOF – synthesis – sorption

## Context

In the scope of carbon mitigation, the **capture of $CO_2$** accounts for most of the energy requirement in a carbon capture and sequestration (CCS) chain. Thus, finding **novel means to significantly reduce this capture energy** can open gateways to deployment. One can equally consider estimations concerning the future energy mix with the International Energy Agency suggesting that the needs for gas will increase by around 1.9% compared to only 0.6% for petrol. Furthermore, the advantage of using natural gas is that a natural gas combined cycle emits around 4% $CO_2$ with respect to other sources such as coal (15%). The recovery of $CO_2$ from streams of such low concentrations is not trivial and the chemistry of the capture medium can be expected to play a significant role.

From a capture process perspective, whilst energy use is critical, other parameters of importance include installation footprint and effects on the environment. In these respects, an **intensified adsorption-based capture approach** can be of interest with respect to standard amine scrubbing. The team at **TOTAL-PERL is evaluating a rapid capture-release process** where the role of water is central. Whilst the current process and adsorbent are acceptable for flue gases where the $CO_2$ concentration is above 10%, it is not the case for low concentrations.

**The aim of this project is to explore novel sorbents that can capture low concentrations of $CO_2$ from $N_2$ and $O_2$ in the presence of humidity**. Further constraints include stability to oxidation and to steam at 120°C. Amine grafted materials may not provide the optimal solution. In this context, the use of **Metal-Organic Frameworks (MOF) has arisen as a promising alternative**. Indeed, due to their unprecedented high versatility and modularity, their crystalline hybrid porous structure can be finely and wisely tuned, in terms of chemical and geometrical features, to meet to most suitable specifications allowing the best compromise between performance, sustainability and energy-efficiency.

## Scope of work and objectives

This project will be carried out at the Institut des Matériaux Poreux de Paris (ESPCI, ENS, Paris) with a close collaboration with the research team at TOTAL-PERL (Lacq). The candidate will also have the opportunity to visit the PERL site in order to visit the testing facilities and discuss the results.

The **objectives of this work** focus on:

(i) the **exploration of a preselection of MOFs**. **Synthesis optimization** (at the g-scale) and **chemical modification** of the materials will be also explored;
(ii) the **characterization of materials** by means of Powder X-ray diffraction, IR spectroscopy, thermo-gravimetric analysis, gas ($N_2$, $CO_2$) and vapor ($H_2O$) sorption and SEM-EDX.
(iii) the **evaluation of materials** will be carried out at TOTAL-PERL by staff at the site. This will include $CO_2$, $N_2$, $O_2$, $H_2O$ isotherms at various temperatures in order to evaluate uptakes, selectivities and stability as well as multicomponent breakthrough experiments in the presence of $H_2O$ for kinetics and competition. Post-mortem evaluation of the materials may be performed at both sites.

## Expected skills

The candidate is expected to show the following skills:

- Dynamic and proactive;
- Ability to analyse the data;
- Ability to work independently;
- Good English level (oral, written);
- Strong communication skills;
- An experience in MOF (or porous solids) synthesis, characterisation and/or and shaping will be appreciated.

## Additional information

**Project host:** Institut des Matériaux Poreux de Paris, UMR CNRS 8004 ESPCI, ENS, 10 rue Vauquelin, 75005 Paris.

**Level of degree:** Master (graduate).

**Project duration:** 6 months.

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