PhD proposal
Research laboratory: LTEN
Closing date for applications: June 15, 2024
Starting date of the PhD: 1st October 2024

TITLE OF THE DOCTORAL RESEARCH PROJECT: Optimization and thermal management of CO2 capture using graphite-MOF composites at various scales (from material to industrial process scales) using experimental and modelling approaches.

Whole context of the PhD program:
The PhD project is a part of the national 4 years TEM-MOF ANR ongoing research program led by the IMN laboratory and shared with LTeN and ICMN partners. The PhD student will be member of the LTeN Nantes University / CNRS laboratory and will collaborate with the different members of both IMN and ICMN labs involved in the TEM-MOF project.
The PhD salary and research costs will be fully covered by the ANR TEM-MOF funding.
The PhD student will be enrolled in the SIS PhD School of Nantes University and will be submitted of both rules of the SIS PhD School and the LTeN lab.

Research subject:
In the context of the Energy transition, and more specifically to contribute to the SNBC national strategy, efficient and sustainable CO_2 capture technologies and related materials are highly expected. For both CO_2 capture from atmosphere or industrial process, adsorption approaches using super-adsorbent such as emerging MOF materials (Metal Organic Frameworks, see Figure 1) offer promising perspectives. Nevertheless, under industrial operating conditions, the effective storage capacities of those materials are significantly reduced (up to 50%) by induced thermal effects (heat of adsorption and heat of desorption) also responsible for reduction in selectivity, even hot spots hazards. Moreover, the energy consumptions of the regeneration of those adsorbents still need significant reduction to reach more advantageous costs and better sustainability.

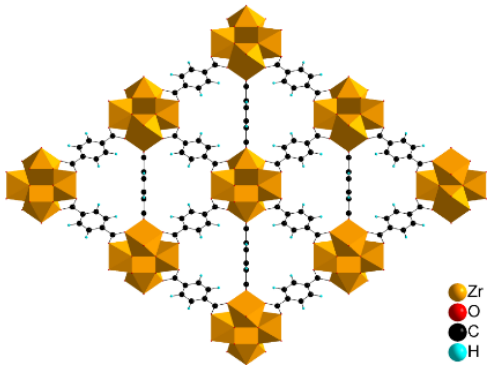

Figure 1. Crystal structure of the MOF UiO-66 or $Zr_6O_4(OH)_4(BDC)_6$(BDC=1,4 benzenedicarboxylate)

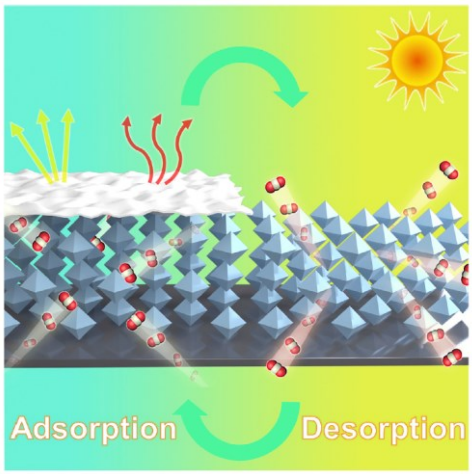

Figure 2. CO_2 capture thermally driven by both radiative cooling (adsorption) and solar heating (desorption).

The three main objectives of the TEM-MOF pre-proposal project are focussed on those critical issues and can be summarized as follow: **(1) to enhance the CO_2 effective capture capacities of MOF adsorbents by a proper thermal management, (2) to optimize the regeneration step by efficient thermal management and (3) to reduce the energy cost of the thermal regeneration**.

The PhD program is focused on the assessment and optimization of the thermal management of CO_2 capture using graphite-MOF composites at various scales (from material to industrial process scales) by complementary experimental and modelling approaches.
A first experimental device will be used to study at the composite scale the heat transfer mechanisms and efficiencies of various G-MOF composite configurations under adsorption and desorption steps, to compare at this scale various possible thermal regeneration techniques, the MOF adhesion on graphite support and the aging of composites under cycling.
Those experiments will be completed with corresponding numerical models needed for a better understanding and control of the CO_2/G-MOF system, for the composite composition and configuration optimisation and for the column size following model.
A second experimental work is focused on two different devices adapted to atmospheric CO_2 capture and industrial flue gas CO_2 capture respectively. A design for atmospheric CO_2 capture panel thermally driven by a solar and radiative-cooling will be designed (Figure 2), implemented and then tested.
A lab scale column will be designed and implemented to test the various G-MOF composites under adsorption and desorption steps at various operating conditions (temperature, pressure, flow rates).
Both CO_2 capture applications (atmospheric and industrial flue gas CO_2 captures) will be modelized for a better understanding and assessment of the obtained results, for optimization and further scale-up.

Supervisors and Contacts:

The PhD will be supervised by two permanent researchers of the LTeN laboratory, namely Pr Xavier PY and Dr Elissa EL RASSY, the involved student will also participate to the ANR TEM-MOF meetings and to the corresponding reports.

Contacts :

- xavier.py@univ-nantes.fr: doctoral research director
- Elissa.elrassy@univ-nantes.fr: doctoral research co-supervisor

Candidate profile:

Engineer and/or Master.
Motivation for research activity with a coherent professional project.
Good level of general and scientific knowledge.
Good level of French (daily communication) and English (bibliography and dissemination of scientific culture).
Analysis, synthesis, innovation and communication skills.
Qualities of adaptability and creativity.

Prerequisites (specific skills for this thesis):

For this doctoral thesis subject, the successful candidate must have strong skills in heat transfer, materials science, and process engineering, but also be able to develop numerical simulations (Comsol Multipysics®, Matlab, etc.) in support of experimental developments.

Location of the thesis:

Nantes Thermal and Energy Laboratory (LTeN), UMR CNRS 6607
Polytech'Nantes, Rue Christian Pauc, 44303 Nantes Cedex 03

To apply :

Send your file to theses.doctorat-bretagneloire.fr including:

1. a detailed curriculum vitae
2. a motivation letter
3. L3, M1, M2 transcripts
4. a copy of the identity card or passport
5. The names and contact details of at least two people who can be contacted for recommendations

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