PhD POSITION (3 years)
Labs: RAPSODEE (Albi), LPCNO (Toulouse), LCC (Toulouse)

Title: "PhD. Synthesis of alternative fuels by the direct hydrogenation of carbon dioxide: Development of cooperative catalysts based on isolated metal atoms and nanoparticles, and environmental assessment of the production process"
PhD supervisors: Doan PHAM MINH, Yasmine LALAU, Katerina SOULANTICA, Philippe SERP
Keywords: Single atom catalyst, nanoparticles, supported catalysts, CO_2, Fisher-Tropsch synthesis, alternative fuels

Environment of the position:
IMT MINES ALBI is part of the Mines-Telecom Institute, which is today the first group of schools of engineering and management in France. IMT Mines Albi is also an associate member of the Federal University of Toulouse Midi-Pyrénées and a partner of a great number of institutions and prestigious universities in France and abroad. These privileged partnerships make it a welcoming 'grand école' and research center, rich in opportunities, and in economic and professional development prospects. Joining IMT Mines Albi means being part of this network and benefiting from its expertise and the wide variety of opportunities it offers.
This PhD position is open at the IMT MINES ALBI, and attached to its RAPSODEE research center (UMR CNRS 5302) with 105 people (permanent and non-permanent staff). The main activities of the lab are structured into two research groups in the fields of energy, environment (group EE) and powder and process (group PP). For more information: https://www.imt-mines-albi.fr/rapsodee/.

Context:
Synthetic alternative fuels play an important role in the defossilization of future air-transportation. One of their important advantages is their compatibility with the existing infrastructures and fleets. This collaborative project involves three laboratories (LCC and LPCNO, Toulouse and RAPSODEE, Albi) and an industrial group (Altens), and aims to produce alternative fuels by the direct hydrogenation of CO2 via CO2-Fischer-Tropsch synthesis (CO2-FTS), which takes place through two consecutive steps: (i) the hydrogenation of CO2 to CO (RWGS: reverse water-gas shift), and (ii) the subsequent hydrogenation of CO to hydrocarbons (Fisher-Tropsch synthesis: FTS).

PhD program:
For this, an innovative concept in catalysis is proposed. The catalysts envisaged combine both metal single atoms allowing the transformation of CO2 into CO and metal nanoparticles catalyzing the FTS at a low temperature range (220-250°C). This will be achieved through the complementary skills of the partners in: i) material chemistry (LCC, LPCNO, and RAPSODEE) that will undertake the synthesis and the characterization of catalysts; ii) process engineering (RAPSODEE) for the engineering of catalytic processes, as well as for the environmental and economic analysis of this new way of production; and iii) alternative fuels (Altens). Different catalytic configurations of CO2 reduction will be studied, with a particular attention to the optimization of the reduction of CO2 in CO and of the FTS for an efficient coupling of these two reactions in a single reactor. Thus, new innovative supported catalysts combining both metal Single Atom Catalyst (SAC) and nanoparticles (NPs) in a controlled way will be synthesized. The idea is to design SAC-NPs cooperative catalysts, which facilitate reaction pathways that would be less favorable with only one type of site (SAC or NPs) for Fisher-Tropsch synthesis. A large variety of techniques (TEM, STEM-HAADF, EDX, HREM, N2 adsorption, chemisorption, XPS, FTIR, Raman and XRD) will be used for the characterization of the catalysts. These catalysts will be evaluated in Fisher-Tropsch synthesis using a fixed-bed reactor, and appropriate analysis systems. The most interesting catalysts will be tested in a

pilot (fixed-bed reactor of 35 mm of internal diameter). Note that preliminary results on the feasibility of direct CO2-FTS have already been obtained by the 3 academic partners of this project.

The development of a catalyst and the associated catalytic process are the main challenges of the project, in order to provide a more efficient process with a longer lifespan than current solutions. The challenge is also to make this technology viable. To make the assessment, the environmental relevance will be assessed via a Life Cycle Analysis (LCA) which will quantify the impacts of the fuel produced. A first economic estimate will also be made, for a multi-criteria evaluation of technical innovation. The success of this project would constitute an important technological brick to a green transportation sector.

The work will be conducted in the three laboratories (RAPSODEE, LCC and LPCNO). Short stays in the local of the industrial partner will also take place.

Application:

The ideal candidate should have solid background in inorganic chemistry or materials science, as well as experience in nanochemistry and/or heterogeneous catalysis. This ambitious 3-years PhD project will offer to the PhD student the opportunity to acquire a solid experience in nanomaterials and supported catalysis.

Applications should include a detailed Curriculum Vitae, a motivation letter, academic transcripts, and at least a recommendation letter.

Deadline for application: July 15th, 2022.

Employer: IMT Mines Albi.
Gross salary: 2090 € per month (net salary: 1680 €).
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