



Interfacial ionic liquid-based heterogeneous catalysts for low temperature CO₂ reduction

Efficient CO₂ conversion using green H₂ coming from renewable sources can contribute to reduce CO₂ emission in order to limit global warming. However, finding efficient catalysts able to operate under mild conditions is critical. This project aims to rationally design a new generation of innovative supported catalysts for CO₂ hydrogenation, combining supported metal nanoparticles and a task-specific ionic liquid (IL), in order to achieve interfacial IL-based catalysis for low temperature thermal CO₂ reduction. Ionic liquids specifically optimized for this purpose will be designed with a supervised machine learning (ML) framework, which will link relevant theoretical and experimental descriptors with experimental catalytic activity and product selectivity. The catalysts resulting from ML as well as the most promising catalysts from the screening will be tested and involved in long-term stability tests.

The recruited PhD will work on the preparation of supported catalyst by conventional as well as by “chimie douce”, their characterization by several techniques (TEM, XPS, XRD, TP-methods,...) and their use in the CO₂ reduction. The obtained results will be used for training the ML algorithm. In a second step the best catalysts resulting from the screening phase of ML will be prepared and tested.

The thesis work is part of a collaborative ANR project involving an industrial partner. The project involves another doctoral student (theoretical chemistry & ML) and one post-doctoral student (organic chemistry and ILs), all located in Toulouse (LCC, LPCNO and Solvionic).

Interested candidates should send a CV, a letter of motivation, at least one recommendation letter, and the names of 1-2 references to philippe.serp@ensiacet.fr and ksoulant@insa-toulouse.fr.

Experience acquired

This ambitious 3-years PhD project will offer to the PhD student the opportunity to acquire a solid experience in (i) catalyst preparation and characterization, (ii) heterogeneous catalysis, (iii) nanoparticles synthesis by colloidal methods. Furthermore, knowledge in organic chemistry and machine learning will be acquired through the strong interactions of the hired PhD with the PhD working in theoretical chemistry & ML and the post-doc working on IL.

Application

The ideal candidate should have solid background in inorganic chemistry or materials science, as well as experience in heterogeneous catalysis.

Starting date: 1st October 2023

Deadline for application: July 1st, 2023.

Employer: CNRS.

Gross salary: 2135 € per month (net salary: 1777 €).

Contact: philippe.serp@ensiacet.fr and ksoulant@insa-toulouse.fr.