BI-OINSPIRED CATALYSIS FOR THE CAPTURE AND VALORIZATION OF CO_2 USING SUPERCRITICAL CONDITIONS

Level : PhD

Profile of the candidate : Good skills on organic, inorganic and organometallic synthesis. Chromatographic and spectroscopic analysis (GC, NMR, IR, UV…) and related software. Hold a Master of Chemistry degree with at least 5 months internship in a research laboratory. Good marks during chemistry studies (bachelor & master) are required to get a "Ecole Doctorale de Chimie de Lyon" grant.

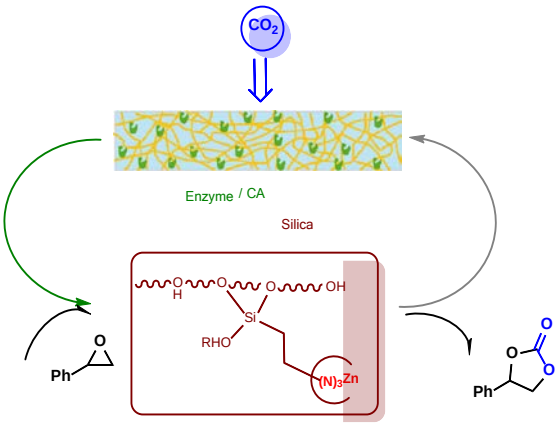
Team(s) : C'Durable and Ingénierie

Contact(s) : Dr. Lorraine CHRIST Lorraine.christ@univ-lyon1.fr , Dr. Alain TUEL

Keyword(s) : Homogeneous and supported catalysis, CO_2 reactions, Green chemistry

Scientific context : Even if anthropic carbon dioxide excess in earth atmosphere is a problem, this waste could be regarded as a largely available carbon source. The use CO_2 as a valuable substrate is actually an important challenge since its catalytic transformations can lead to valuable products such as urea, carboxylic acids, carbamates and carbonates. Organic carbonates are very useful compounds that can be linear (DMC, polycarbonates) or cyclic (solvents for Li batteries). Our recent studies focus on the preparation of cyclic carbonates from the cycloaddition of CO_2 to epoxides, catalyzed by zinc complexes[1]. Moreover, this total atom economy reaction doesn't need any organic solvent since CO_2 can be the solvent under supercritical conditions (>80 bar).

Missions & Outlook : The capture of CO_2 can be achieved by amine based processes or enzymatic reactions. We developed a capture procedure based on carbonic anhydrase[2] that we will now couple to the CO_2 zinc catalyzed cycloaddition to epoxides. As the enzymatic step is reversible, the driving force of the global process leads on carbon dioxide transformation; the rate of the CO_2 cycloaddition to epoxides can be significantly increased using supercritical conditions[3] which can be monitored in a sapphire glass lined reactor. The main challenge of this PhD proposal is to find the specific conditions that will allow the coupling of both steps since the enzyme do not stand temperatures above 60°C. This can be achieved by tuning the CO_2 pressure and epoxide amounts but also by modifying the zinc catalyst and using a bioinspired histidine complex. The second challenge is to fix the catalysts in a silica support to get a recyclable system by grafting them *via* $Si(OR)_3$ groups[4].



Bibliography

1.- L. Christ *et al. J.CO2 Utilization* **2021** https://doi.org/10.1016/j.jcou.2020.101380
2- L. Christ, A. Pierre *et al. J. Mol.Cat. B: Enzymatic* 2009, **60,** 163
3- M. Djoufak, *PhD thesis*, Université Claude Bernard, Lyon 1, **2013,** pp 124
4- A. Tuel *et al. New* J. Chem. **1999**, 23, 473