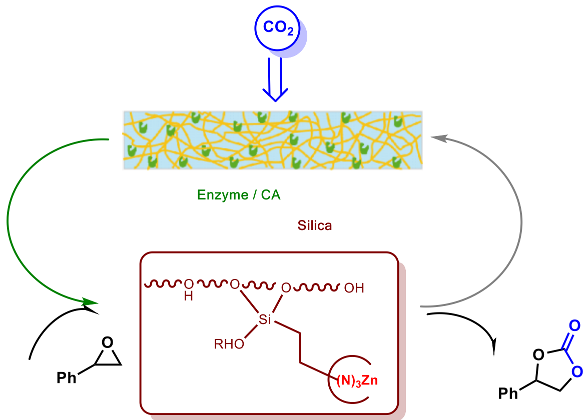
Bioinspired catalysis for the capture and valorization of CO_2 using supercritical conditions

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, polymer precursors). Our recent studies focus on the preparation of cyclic carbonates from the cycloaddition of CO_2 to epoxides, catalyzed by chromium or zinc complexes[1]. Moreover, this total atom economy reaction doesn't need any organic solvent since CO_2 can ensure this behavior when using supercritical conditions.

Project

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 both catalysts in a silica support to get a recyclable system that could be used in a fixed bed reactor to get a continuous process. The zinc species will be grafted *via* $Si(OR)_3$ groups[4] while the encapsulation of carbonic anhydrase will be achieved by sol-gel synthesis and supercritical drying to form stable aerogels[5].



References

1- L. Christ *et al. J. Mol. Cat. A: Chemical* **2013**, 381, 161 & *Molecular Cat*. **2018**, 456, 87
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
5- L. Christ, A. Pierre *et al. Applied Catalysis*, A: General**, 2008,** 344, 70

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Skills

Organic, inorganic and organometallic synthesis. Handling of pressurized stainless steel reactors. Chromatographic and spectroscopic analysis (GC-FID, NMR, IR, UV-Vis).

Application

Candidates should hold a Master of Chemistry degree with at least 5 months internship in a research or industrial laboratory. Speaking basic French is required. Send a CV and recommendation letter(s) to Dr. L. Christ before 27-05-2019. **Salary:** ~1300 €/month over 36 months, starting: October/November 2019.

Supervisors

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