Master 2 internship in Chemistry

Towards the tuning of the selectivity of electrode integrated molecular catalyst through molecular surface engineering

Abstract : Despite the recent and rapid development of molecular catalysts for the electrochemical reduction of CO_2, the control of the selectivity of the metal centre remain limited to the understanding of the effect of the surrounding ligands and functional groups that they bear. This imply demanding synthetic steps which makes these promising molecular approaches less likely to reach a potential technological maturity.
In this project, we will aim at modifying the direct environment of the molecular catalyst through co-immobilisation of targeted functional groups that should allow to modify the electrochemical and electrocatalytic activity of the confined catalyst.
Starting with a known cobalt containing catalyst previously developed in the SolHyCat team at the LCBM lab, this internship thus target the development of original multifunctional electrode surfaces which should allow us to further understand how to control and tune the activity and selectivity of adsorbed catalysts in the context of small molecule activation for energy conversion.

Objectives: The main aim of this internship is to control the assembly of a variety of surface functions, through non-covalent grafting, at the surface of carbon nanotube electrodes and co-immobilised with a CO_2-reduction molecular catalyst. Through a range of electrochemical characterisation techniques, the molecular assemblies will be tested to probe the impact of the catalyst environment on the selectivity of the catalytic process.
Within the course of this internship, the student will have the opportunity to gain specific experience in the area of surface functionalisation and electrochemical/catalytic characterisation of multifunctional surfaces. Along with these main surface functionalisation and electrochemical investigation, the internship will also include the synthesis and characterisation of novel derivatives to anchor at the electrode to assist the catalyst during turnover.
The internship will involve organic (and inorganic) synthesis methods and standard characterisation techniques (NMR, IR, UV-vis), preparation of carbon nanotube-based electrodes through various methods (ink deposition, film phase transfer), surface modification and characterisation (UV-vis, IR-ATR) with a focus on the electrochemical characterisation. Products of the electrolysis will be analysed by gas and ionic chromatography and NMR.

Expected skills: The applicant should have some knowledge in organic synthesis, catalysis and a great interest for surface functionalisation for electrocatalysis and energy conversion. Basic knowledge in electrochemistry would be a plus.

Period: January/February to June/July (anticipate 3 month prior to the start of the internship in order to complete the CEA administrative tasks). Possibility of continuing on with a PhD contract conditioned to funding availability.

The laboratory: The Laboratory of Chemistry and Biology of Metals (LCBM) hosts a diverse community of researchers, from biologists to chemists, studying the role of metals in biological systems (cells, metallo-enzymes) as well as their use in the development of fully synthetic systems for health and energy applications. More specifically, over the past decade the SolHyCat team has built a strong expertise in the design of bio-inspired catalysts and photosensitizers as well as their grafting at (photo)electrodes surfaces in order to further study these molecular systems in operational conditions in proof-of-concepts functional devices.

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