



**Research Doctorate (Ph.D.) in Chemical Sciences**  
**32<sup>nd</sup> Cycle – Academic Year 2016/2017**

**Tutor:**

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**Project Information**

**1 - Title**

From catalytic cycles to material properties: development of an integrated experimental and theoretical approach.

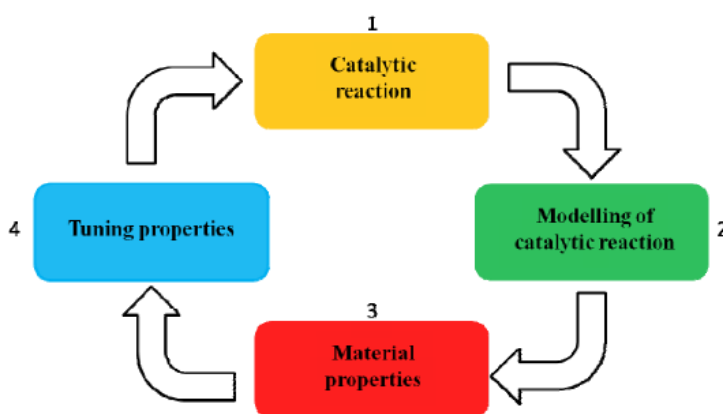
**2 - Key words**

1. Catalytic cycle
2. Material properties
3. Computational modelling
4. Industrial reactions
5. Tuning design of material properties

**3 - Abstract**

Aim of this proposal is the development of a combined experimental and theoretical approach for catalytic reaction of industrial interest to obtain targeted materials.

We will focus on ring opening polymerization of poly(lactide) (PLA) as well as copolymerization of CO<sub>2</sub> and epoxides that meet an considerable current interest because they are producing biodegradable thermoplastic as well as the CO<sub>2</sub> fixation. The ring opening polymerization (ROP) mechanism will be investigated by using DFT calculations in order to find a relationship of catalyst structure with the polymer microstructures. Several PLAs samples will be characterized in terms of physical and mechanical properties in order to correlate the polymer microstructures with the desired properties. The iteration of this catalytic cycle should lead to a "catalyst design" with "targeted materials".



Scheme 1