



***Ph.D. School in Chemical Sciences
Cycle XXXVIII***

Proposer: *professor Giovanni Talarico*

Research project title: Following the transition from conventional plastics to biodegradable materials by a combined experimental and theoretical approach

Key words Circular economy; biodegradable materials; polymerization catalysis; DFT calculations

Research project abstract: One of the most important goals in the modern society is to deplete the usage of fossil fuels and the optimization of biodegradable materials is essential for reducing the carbon footprint. However, polyolefins still represent the election material for many applications due to the optimization of polymerization catalysis witnessed over the past decades. This PhD project aims to move the knowledge developed on olefin catalysis to a fast and efficient methodology for stereoselective catalysts of biorenewable sources. The enantioselective catalysts for the ring opening polymerization of lactides and the copolymerization of CO₂/epoxides will be targeted by a three-step methodology relying on i) computational "reading" of catalysts properties based on steric and electronic descriptors; ii) mechanistic validation by polymerization kinetics and DFT modeling and iii) "mechanism-driven" database to be used to accelerate catalyst design for the targeted applications.