CATCHEMPRO

Contributions to Catalysis towards Sustainable Chemical Production

Timeline | 01/2020 to 12/2022

Budget | 229,900 €

ICIQ People | Pericás Research Group

Call | Proyectos I+D - Retos Investigación 2019

SUMMARY

The project "Contributions to Catalysis towards Sustainable Chemical Production (CATCHEMPRO)" builds on previous research efforts of the Pericàs lab in the 2009-2019 time frame centered on the development of immobilized catalysts for the production of enantiopure compounds in batch and flow. We now aim at completing ongoing studies in this area with the ultimate goal of developing catalytic solutions in the fields of metal catalysis and organocatalysis towards the paradigm change from batch to flow for a more sustainable chemical production.

Progress towards this global objective will be achieved through work in five different areas (WPs): i) Development of new, robust immobilized catalysts allowing the development of practical continuous flow versions of relevant chemical processes. ii) Ex-novo development of metal-catalyzed processes through processes involving high throughput experimentation (HTE) guided discovery, optimization, ligand modification for immobilization and, finally, implementation in continuous flow. In this area, special emphasis will be put on photocatalytic flow processes with immobilized species. iii) Development of a practical procedure for the synthesis of cyclic organic carbonates (COC) from carbon dioxide in continuous flow. iv) Understanding the role of anion-pi interactions in photocatalysis, and realizing their synthetic potential. v) Understanding and harnessing the synthetic potential of the Ni(0)/aminophosphine catalytic system.

In WP1, new immobilized organocatalysts acting through non-covalent activation mechanisms will receive special attention. In WP2, we will strive for integrating in silico screening and high throughput experimentation for the accelerated discovery of (photo)catalytic reactions. The use of immobilized catalysts will be incorporated at early stages of these processes, with the ultimate goal of converting the reactions discovered through this procedure into continuous flow processes. In WP3, we will aim at developing a practical continuous flow process, operable near room temperature and atmospheric pressure, for the conversion of carbon dioxide and epoxides into cyclic organic carbonates (COC). Attention will be paid to technological aspects of the gas liquid reaction, to the kinetic resolution of racemic epoxides, and to the implementation of a process allowing the conversion of crude glycerol from biorefineries to COC. In WP4, we plan to work on identifying photochemical processes likely taking place through activation by anion-pi interactions, and characterizing these processes by photophysical and theoretical studies. Two additional tasks will be the development of synthetic applications of amidyl radicals generated by photochemical processes involving anion-pi and exploring functional classes of organic compounds involving weak covalent bonds in their functional groups as potential candidates for photochemical activation through anion-pi. In WP5, we plan to explore new applications of the Ni(0)/aminophosphine system that we have recently introduced for reductive [2+2] cycloadditions of alkynes. In particular, the development of an asymmetric version of the reaction will be pursued, as well as a modified version of the reaction allowing the preparation of cyclobutenes bearing quaternary carbon centers. In addition, we plan to intercept with carbon monoxide one of the putative intermediates leading to the cyclobutene, diverting in this way the pathway towards cyclopentadienones.

Reference: PID2019-109236RB-100