EnergyCat

Molecular Redox Catalysts for Green Energy Applications

Timeline | 09/2023 to 08/2023

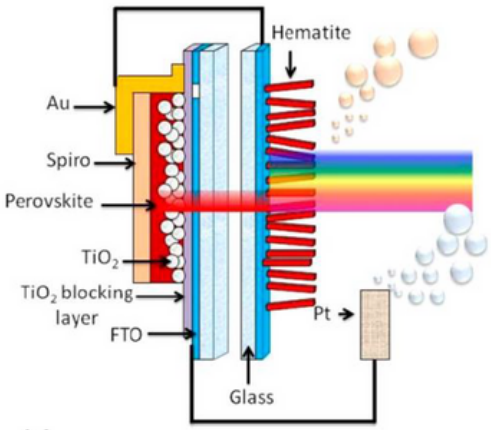
ICIQ People | Llobet Research Group

Budget | 312.500 €

Call | Proyectos I+D - Generación Conocimiento 2022

SUMMARY

The main objective of **EnergyCat** is to create efficient hybrid molecular materials as electrodes and molecular photoelectrodes for redox reactions that significantly improve the cutting-edge materials available today. This will be achieved through a detailed knowledge of the kinetics and thermodynamics of the multiple chemical reactions that govern their behavior. We propose to develop and optimize each of the components necessary to achieve this objective. In particular, we propose to enhance key reactions such as the oxidation of water and ammonia to molecular oxygen and nitrogen, respectively. On the reduction front, we will address the transformation of CO2, especially in the achievement of products beyond CO. All catalysts used in this project will be based on transition metal molecular complexes. The best catalyst obtained here will be anchored later on conductive surfaces to carry out molecular electrocatalysis. The anchoring will be carried out through different types of interactions between the surface and the molecular species and those oligomeric and polymeric transition metal complexes will be privileged. In addition, the best catalysts anchored in semiconductors that will allow us to carry out the corresponding reactions for the decomposition of water and the reduction of CO2, induced by sunlight. To this end, we plan for careful development of transition metal molecular complexes capable of overcoming the inherent challenges of these reactions. These involve multiple electron and proton transfers and thus access to multiple oxidation states. To rationally design the molecular nature of these catalysts we will carry out reactivity studies, kinetic analysis and isotopic labeling to establish the reaction mechanisms through which these reactions occur. This will allow us to determine the nature of the slow steps from the set of reactions that take place in the corresponding catalytic cycles. In this context, it will also be critical to clarify the set of reactions that lead to non-productive processes or reactions that lead to the derailment of the catalytic cycle that generates unwanted or decomposition products. A set of conducting and semiconducting surfaces has been judiciously chosen to anchor the catalysts that will be developed in this project. These include graphitic type materials as well as oxides depending on the nature of the experiments to be carried out. The study of the interaction between the molecular catalyst and the surface will be one of the key factors to guarantee the correct functioning of the hybrid material. This development is expected to lead to highly efficient materials for the photochemical generation of clean and sustainable solar fuels.



Reference: PID2022-140143OB-I00