CatFuel

Development of Molecular Catalysts Relevant for Solar Fuels Generation

Timeline | 06/2020 to 05/2023

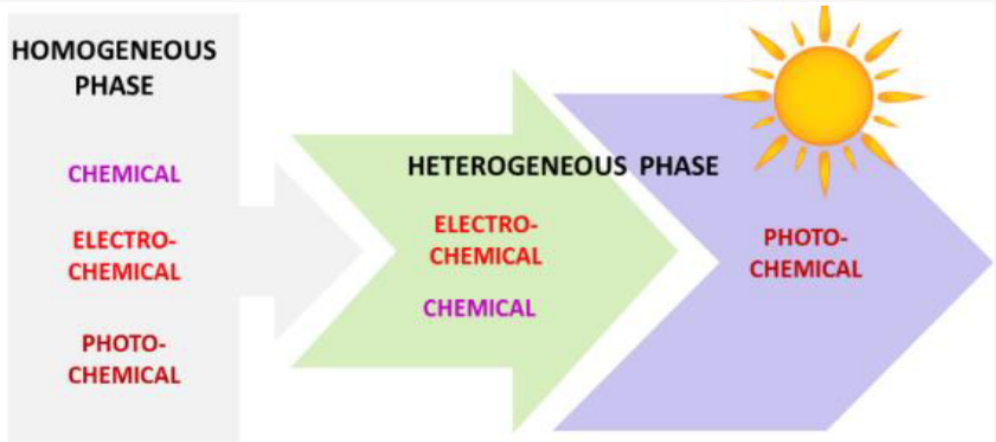
Budget | 254,100 €

ICIQ People | Antoni Llobet Research Group

Call | Proyectos I+D - Retos Investigación 2019

SUMMARY

The main objective of the project is to come up with hybrid molecular materials that efficiently work as photoanodes and photocathodes and that significantly improve todays available state of the art materials. This will be achieved via a detailed knowledge of kinetics and thermodynamics of the complex chemical reactions that govern their behavior. We propose to develop and optimize each of the components necessary to achieve such objective. In particular, we propose to improve key reactions such as oxidation of water and ammonia to molecular oxygen and nitrogen respectively. On the reduction front we will deal with transformation of protons to hydrogen and CO_2 to methanol and methane. All the catalysts used in this project will be based on molecular transition metal complexes. The best catalyst obtained here will be later on anchored on conductive surfaces in order to carry out molecular electrocatalysis. Further, the best catalysts anchored on semiconductors will allow us performing the corresponding light induced water splitting or CO_2 reduction reactions. For this we plan a careful development of molecular transition metal complexes capable of dealing with the inherent challenges of these reactions; these involve multiple electron and proton transfer and thus access to multiple oxidation states. In order to rationally design the molecular nature of these catalysts we will carry out reactivity studies, kinetic analysis and isotopic labeling in order 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 the elucidation of the set of reactions that lead to non-productive processes or reactions that lead to derailment from the catalytic cycle generating undesired or decomposition products. A set of conducting and semiconducting surfaces has been judiciously chosen to anchor the catalysts to be developed in this project. Those include graphitic type of materials as well as oxides and chalcogenides depending of the nature of the experiments that will be carried out. This development is expected to lead to highly efficient materials for photochemically driven generation of solar fuels.



Working strategy flow chart

Reference: PID2019-111617RB-100