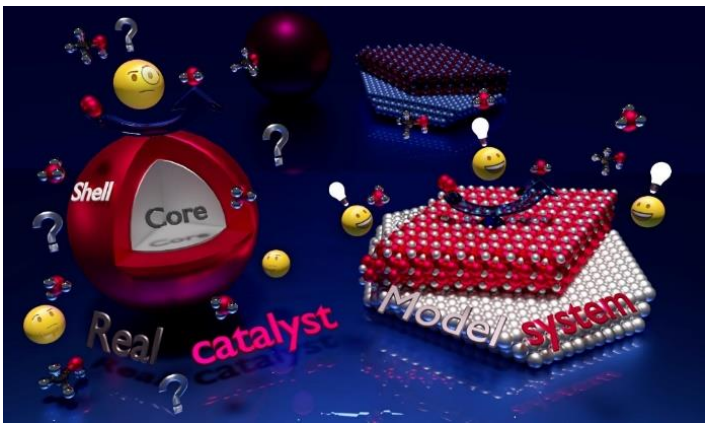

The study of new materials for energy storage and conversion is a priority of modern scientific and technological research because it responds to the current, important needs of society in the context of the development of ***sustainable energy based on alternative and renewable sources***. In this regard, the efficient conversion of chemical energy into electricity and *vice versa* requires the development of innovative electrocatalysts for use in fuel cells, battery and electrolyzers, which are currently optimised through the empirical "trial&error" method. Under this project, **a knowledge-based approach will be used in conducting basic research using state-of-the-art surface science techniques** in order to understand the effect of the key interfacial phenomena typical of matter at the nanoscale, such as *interfacial electronic hybridization, electron tunneling and steric confinement* on the electrocatalytic activity. Surface science approach will provide insight into the properties and processes taking place at the solid-liquid interface at the ***atomic level*** and under the ***operational conditions***, focusing on the electrocatalytic reactions of the evolution of hydrogen (HER), which is the bedrock of the nascent hydrogen economy and the oxygen reduction reaction (ORR) as a lateral reaction of the cathode for the application in fuel cells. Commonly used materials nowadays for efficient catalysts are platinum or palladium, elements with the best catalytic properties, but their high cost and low resources of any metals from the Pt-group still remain an issue in order to implement them in fuel cells and the production of oxygen or hydrogen by electrolysis on the global market. Therefore, several strategies are currently pursued (Pt alloys, nanostructured and core-shell catalysis, non-Pt group metals, transition metal carbides, halides or nitrides and phosphides) in order to reducing Pt loading or complete replacement of precious metals while maintaining or even increasing the efficiency of these devices.

The project aims to investigate model systems reflecting core-shell type nanostructured electrocatalysts based on 2D materials such as graphene, N-doped graphene and transition metal chalcogenides (TMDC), which have been shown to have not only excellent intrinsic electroactivity, but also take participation in important phenomena at the nanoscale if they are deposited on substrates of transition or noble metals. These properties are not available when these materials are used separately. Phenomena such as **electron tunneling, interfacial hybridization and steric confinement**, can be used for the rational design of advanced catalysts with radically improved parameters and properties. Moreover, 2D materials can be chemically modified by introducing single atoms forming the so-called *single* **atom catalysts** (SAC), characterized by unconventional coordination and electronic structure, which often have quite a unique chemical activity.

The objective of this project is to **precisely define the relationship between catalytic activity and material structure at the atomic level** through a rigorous approach, based on the synthesis of model systems under ultrahigh vacuum (UHV) conditions (2D thin films supported on single crystals) and using advanced and complementary in operando and in situ techniques, such as Electrochemical Scanning Tunneling Microscope (EC-STM), Raman spectroscopy and X-ray photoemission spectroscopy (XPS). This innovative methodological approach combines microscopic techniques capable of identifying catalytically active sites and their structures with atomic precision, with spectroscopic methods that are sensitive to changes in chemical and electronic states caused by the direct and indirect effects of the electrocatalytic reaction. This approach will allow to determine: ***i) reaction pathways and selectivity drivers; ii) 2D materials activation mechanisms based on electronic effects or chemical phenomena in confined space and hybridized surface; iii) mechanisms of degradation and transformation of materials under the operating conditions of the catalyst.*** The planned research is of an *interdisciplinary nature*, combining several fields of science, such as physics, chemistry, nanotechnology and materials engineering, which are crucial for the rational design of modern, highly efficient electrocatalysts.