SMELT

Simulations of dynamic materials for photo-electro-catalytic processes

Timeline | 09/2022 to 08/2025

ICIQ People | N. López Research Group

Budget | 181.500 €

Call | Proyectos I+D - Generación Conocimiento 2021

SUMMARY

The specific objectives of **SMELT** are to describe stable, active and selective photo-electro-catalysts for industrially-appealing transformations that can be then applied to the search for optimized materials and/or rules to find new alternative formulations for catalysts with improved performance in terms of activity, selectivity and stability. We aim at employing computational models to help finding new catalytic materials for highly demanded transformations including CO2 conversion, thermal, electrochemical or photoelectrochemical, the oxygen evolution reaction and N2 conversion to ammonia. Due to the complexity of these reactions and to go beyond standard catalytic formulations complex materials that evolve under reaction conditions are needed. These dynamic processes have been mostly overlooked in the past, particularly as they are difficult to address with standard Density Functional Theory and periodic boundary conditions.

However, the appearance of new techniques based on machine learning approaches can be applied to fill the complexity gap in several directions, (i) by providing robust structures that can incorporate dynamic processes, (ii) by allowing the inference of new catalytic descriptors and data-driven equations and (iii) to shorten the gap between modeling and characterization techniques. **SMELT** is built around three work packages: the first one, WP1, is instrumental and devoted to leverage statistical learning tools to applications in photoelectro-catalysis. WP2 is centered on electrocatalysis with OER, CO2 or CO reduction, ammonia synthesis and electrosynthesis; WP3 on thermal and photo-catalysis including CO2 conversion and low-temperature ammonia synthesis. In WP3 the dynamics of charge and a deep electronic structure analysis, which is crucial to energy-related processes characterized by electronic manifolds that allow a low energy demand chemistry but that are very complex to address computationally, will be addressed.

Reference: PID2021-122516OB-I00