MLALH: MACHINE-LEARNING-DRIVEN BOTTOM-UP DESIGN OF ATOMICALLY-LAYERED HETEROSTRUCTURES FOR GREEN H2 PRODUCTION, HA SIDO PROPUESTA PARA FINANCIACIÓN

Description

The field of catalytic green hydrogen production, although indispensable for the transition to a renewable future, still suffers from widespread irreproducibility of results that limits its full commercialisation. The largest obstacle lies in the methods widely employed in synthesising the active catalysts, which impede unambiguously identifying the property-structure relationship. The vast catalytic samples reported in the literature lack uniformity in shape, size, growth orientation of particles, and composition. In an atomically imprecise material, the observed catalytic activity may well be from a subset of the various particles in the sample, which bring about uncertainty in linking the functional properties to a specific atomic level characteristic of the material. This piece of insight is critical for any further improvement in the field.

In this proposal, we will take a fundamentally different path toward predicting, synthesising and characterising catalytic heterostructure for green hydrogen. Our method is theory-guided, where we will screen millions of heterostructures through density functional theory calculations coupled with machine learning for accelerated discovery. We will then synthesise the outstanding prediction usingatomically precise thin-film technology where the composition, growth orientation and thickness of both sides of the heterostructures are atomically controlled. As a result, any macroscale observation can be certainly linked to the heterostructure s atomic-level characteristics.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación