Position Offered: PREDOCTORAL RESEARCHER

Project: *MACHINE LEARNING ASSISTED COMPUTATIONAL INVESTIGATION OF METAL OXIDE CATALYSTS FOR CHEMICAL LOOPING APPLICATIONS*

Technological and scientific fields: New Materials, High Performance Computing, Artificial Intelligence

Location: Valencia, Comunidad Valenciana, Instituto de Tecnología Química (ITQ) https://itq.upv-csic.es/

Research Group/PI: Molecular Design of Catalysts / Mercedes Boronat Zaragozá

PROJECT SUMMARY

In this period of transition towards a sustainable society, it is necessary to develop new technologies for the efficient production of energy and chemicals. In chemical loop processes, a chemical reaction is divided into two separate steps mediated by a metal compound that reacts and regenerates reversibly in cycles, allowing for smoother reaction conditions and energy-intensive gas separation. The design of tailor-made materials for chemical loop applications, based on a deep understanding of the structural evolution of the catalyst under operating conditions, requires the development of new and faster computational methods capable of achieving sufficiently large time and length scales. It is necessary to incorporate Artificial Intelligence techniques and, more specifically, Machine Learning to reproduce the precision of quantum chemistry at a much lower computational cost. The goal of this proposal is to develop accurate machine learning potentials to predict the performance of metal oxides in chemical loop applications. The theoretical study of the thermodynamics and kinetics of such profound transformations of solid materials (complete reduction and oxidation under different conditions) will open up the possibility of making more accurate computational predictions of catalyst behavior under realistic conditions, for these oxides and for other types of solid materials.

PROFESSIONAL PROFILE

Minimum requirements:

Academic qualifications required:

- Bachelor's Degree in Chemistry

Merits to be considered:

Master's degree in Theoretical Chemistry, Materials or related topics, previous experience in computational studies related to catalysis and/or materials, and basic knowledge of programming languages will be valued.

WHAT IS OFFERED

Incorporation into a multidisciplinary group to study the Doctoral Programme in Sustainable Chemistry at the Universitat Politècnica de València (UPV). Learning of computational methods applied to catalysis and machine learning techniques. Two training stays are planned in prestigious research centers. 150 ECTS expected at the end of the contract.

Contract conditions:

Predoctoral Researcher contract of 4 years' duration. Gross annual salary of 23,871.33 €.

Start of contract: before 31 December 2024

PRINCIPAL INVESTIGATOR CONTACT

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