# Position Offered: POSTDOCTORAL RESEARCHER

Project: *Machine Learning Applied to the Catalytic Conversion of Greenhouse Gases into Clean Fuels* 

**Technological and scientific fields:** High-Performance Computing, Artificial Intelligence, Massive Data and Information Processing Technologies, Nanotechnology, New Materials, Climate Change, and Biodiversity

Location: Cantoblanco, Madrid, Instituto de Catálisis y Petroleoquímica, https://icp.csic.es

Research Group/PI: Modeling for Theoretical Catalysis / Pablo G. Lustemberg

## **PROJECT SUMMARY**

In a circular economy, CO2 is valuable for its potential to be reduced with renewable hydrogen, a promising route for the synthesis of fuels and chemical feedstocks. This project aims to develop low-cost catalysts to produce methanol from CO2 and hydrogen. Using machine learning, the design of multicomponent catalysts based on non-noble metals and mixed oxides will be accelerated. The research will combine atomic-scale simulations with artificial intelligence to model and optimize catalysts, understanding reaction mechanisms at the molecular level, in collaboration with leading experimental and theoretical teams.

## PROFESSIONAL PROFILE

#### Minimum requirements:

- Ph.D. in Sustainable Chemistry with a minimum of 2 years of postdoctoral experience.
- Experience in Theoretical Chemistry and Computational Modeling, Density Functional Theory (DFT), and VASP scientific code applied to heterogeneous catalysis.
- Proficiency in English at the C1 level.

#### Merits to be considered:

- Familiarity with the Linux operating system, Python programming, and high-performance computing.
- Experience in interdisciplinary work groups, especially with experimental teams.
- Basic knowledge of machine learning techniques.

# WHAT IS OFFERED

The project focuses on catalyst innovation, specifically on the study of new catalysts. Advanced technologies such as artificial intelligence models (GOFEE and ML-NEB) and molecular dynamics will be employed to accelerate the analysis of these catalysts.

The project will feature prominent international collaborations, fostering an interdisciplinary approach that integrates several theoretical and experimental methods. The training plan includes digital and transversal skills, as well as opportunities for training in international environments through internships. It is planned to obtain 180 ECTS credits at several European institutions, ensuring comprehensive and robust training.

#### Contract conditions:

Indefinite contract for a Postdoctoral Researcher associated to the Momentum Project of 4 years' duration according to Spanish science law. Gross annual salary ( $41.000 \in -52.000 \in$ ).

Start of contract: before 31 December 2024

# PRINCIPAL INVESTIGATOR CONTACT

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