Position Offered: POSTDOCTORAL RESEARCHER

Project: Atomic-Level Study of Tribochemical Processes for Developing New Greenhouse Gas Emissions Reduction Technologies in the Construction Sector

Technological and scientific fields: Climate change and biodiversity

Location: Madrid, Madrid Community, C/Serrano Galvache 4, Eduardo Torroja Institute of Construction Sciences, <u>www.ietcc.csic.es</u>

Research Group/PI: Sustainable Interaction between Construction Materials an Environment, subgroup of Tribochemistry and Triboemissions

PROJECT SUMMARY

The primary goal of this project is to develop groundbreaking technologies aimed at significantly reducing greenhouse gas emissions in the construction sector, with a particular focus on cement manufacturing. The radical innovation lies in the implementation of tribochemical reactions to minimize CO2, CH4, and other emissions. The project proposes exploring entirely novel tribochemical pathways and developing a "one-pot" process for low-temperature decarbonation of minerals and CO2 reduction, which would eliminate the need for costly CO2 capture and storage systems. Specific Objectives include: Determine the atomic mechanisms of tribochemical decomposition in metal carbonates; Determine the atomic mechanisms of active hydrogen generation in tribochemical processes using hydrides, hydrocarbons, agro-forestry residues, etc.; Elucidate the reaction pathways for tribocatalytic reduction of CO2 under H2 atmosphere; Explore tribochemical reaction pathways for direct synthesis of calcium silicates.

PROFESSIONAL PROFILE

Minimum requirements:

- Degree: Doctor of Physics, Chemistry, or Materials Science
- English Proficiency: B2 or higher
- Research Experience: Thesis in computational modeling of physical and/or chemical processes at the atomic level (molecular dynamics, Monte Carlo, Tight-Binding, DFT, etc.)

Merits to be considered:

- Expertise in atomic simulation techniques for mechanical systems (deformation, friction, etc.)
- Postdoctoral experience in highly reputable institutions.
- Participation in research projects.
- High-impact scientific publications with significant candidate's contributions (first author, corresponding author, etc.).

WHAT IS OFFERED

Collaborate within a diverse team: Engage with a multidisciplinary group of researchers, fostering cross-pollination of ideas and expertise.

Immediate Validation of Simulation Results: Leverage the group's experimental capabilities to promptly validate and refine atomic simulation outcomes.

Expanding Expertise in Tribochemical Simulations:

- Cultivate proficiency in advanced, atomic, and quantum simulation techniques (240 ECTS).
- Embark on enriching training stints with renowned groups in the field of tribochemistry;
- Gain proficiency in utilizing first-principles and hybrid methods for model development.
- Access to Cutting-Edge Resources: Advanced Computing Facilities.

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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