Centro de Física de Materiales
Materials Physics Center

POSDOCTORAL POSITION IN THEORETICAL CHEMICAL PHYSICS

CO_2 Capture through Mineralization Studied by Atomistic Simulations and Machine Learning

Contact: Maite Alducin (maite.alducin@ehu.eus)

PROJECT DESCRIPTION

The theoretical *Gas-Solid Interfaces group* and the *Ceramic and Cementitious Materials group* at the CSIC-EHU *Centro de Física de Materiales* (San Sebastián, Spain), invite applications for a joint postdoctoral position in **theoretical and computational research**. The position is associated to the HORIZON 2024 PATHFINDER project,

C-SINC: Concrete products through sustainable and innovative carbon-stored binders

The C-SINC project brings together experimental and theoretical research groups to address the urgent need for decarbonization in cement production by developing alternative binders incorporating CO_2-sequestered magnesium-based silicates, such as olivine and pyroxenes, as supplementary cementitious materials. The ultimate goal is to reduce the embodied carbon emissions of concrete while maintaining or improving its structural performance.

Within this multidisciplinary framework, the successful candidate will contribute to the theoretical work package led by the CSIC Theoretical Team at *Centro de Física de Materiales*. The research will focus on the atomistic mechanisms governing CO_2 adsorption, mineralization, and reactivity in magnesium silicates and related materials. Using state-of-the-art electronic-structure calculations, atomistic simulations, and machine-learning techniques, the postdoctoral researcher will develop predictive models of mineral carbonation processes and provide fundamental insight to guide and complement the experimental activities of the consortium. The position is exclusively theoretical, but the researcher will collaborate closely with the experimental groups involved in C-SINC and will participate in the interpretation and validation of the modeling results against experimental observations.

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CANDIDATE PROFILE

We are looking for a **highly motivated candidate with:**

- A PhD degree in Physics or Chemistry, preferably in the field of Theoretical Chemical Physics.
- Excellent written and spoken English.
- Strong background in Scientific programing (fortran, C++, python, Linux shell scripting…) and in High Performance Computing.
- **Experience in one or more of the following areas**: Density Functional Theory, reactive Force-Fields, atomistic Neural Networks, and Molecular Dynamics Simulations.

APPLICATION PROCEDURE

Suitable candidates are invited to send their application with the following information:

1- A presentation letter with declaration of interests (max. 2 pages).

2- An updated Curriculum Vitae, including a list of publications.

3- Contact details of two potential referees familiar with the applicant's research abilities.

Applicants should send an email to:

Dr. Maite Alducin (maite.alducin@ehu.eus)

Using as email's subject: **C-SINC posdoc**

Deadline: August 31, 2026