

The mission of the Catalan Institute of Nanoscience and Nanotechnology (ICN2) is to achieve the highest level of scientific and technological excellence in Nanoscience and Nanotechnology. Its research lines focus on the newly-discovered physical and chemical properties that arise from the behaviour of matter at the nanoscale. ICN2 has been awarded with the Severo Ochoa Center of Excellence distinction for three consecutive periods (2014-2018 and 2018-2022 and 2023-2026). ICN2 comprises 19 Research Groups, 7 Technical Development and Support Units and Facilities, and 2 Research Platforms, covering different areas of nanoscience and nanotechnology.

Job Title: Postdoctoral researcher (ALCOAT) - First principles studies of the protection of steel against corrosion using scrap aluminium

Research area or group: Theory and Simulation Group

Description of Group/Project: The Theory and Simulation Group has broad experience in developing electronic structure methods and their application to perform atomistic simulations of molecules and materials. These include (but are not restricted to) SIESTA (www.siesta-project.org) and its TranSIESTA functionality. SIESTA is a multi-purpose first-principles method and program based on Density Functional Theory, which can describe the atomic and electronic properties of systems with up to several thousands of atoms. TranSIESTA is an extension of SIESTA that enables the study of electronic transport phenomena in nanoscale devices.

The ALCOAT project proposes using scrap aluminum to protect steel from corroding. The project has a two-fold objective: to propose quaternary alloys with superior anti-corrosive performance while promoting circularity. In collaboration with several experimental and theoretical partners across Europe, the role of ICN2 is to provide atomistic insights into the alloy compositions (containing Fe, Zn, Bi, among others) that maximize the anti-corrosive performance, which perfectly suits SIESTA code capabilities as it can handle thousands of atoms efficiently with ab initio predictability.

The work will be carried out at the Theory and Simulation Group at ICN2.

Main Tasks and responsibilities:

- To run ab initio simulations to predict alloy compositions that maximize anti-corrosive performance.
- To propose models for simulating different alloy phases and interfaces.
- To apply the hybrid QM/MM + NEGF method to consider solvent and voltage effects on the simulations.
- Preparation of scientific reports and journal articles.
- Contribution to other activities in the group.

Requirements:

- **Education:**
PhD in Physics, Materials Science, Chemistry, Computer Science, or related disciplines.

- **Knowledge and Professional Experience:**

Knowledge of programming languages used in data analysis (particularly Fortran and/or python) will be valued but it is not essential.

High Performance Computing.

Experience with High Throughput Calculations will be valued but it is not essential.

Previous experience with SIESTA is essential. Knowledge of SIESTA's QM/MM and TranSIESTA modules (or similar methods from other codes) will be valued, but it is not essential.

Previous experience with SIESTA, including its QM/MM and TranSIESTA modules, is essential.

Other research experience will be considered.

- **Personal Competences:**

Strong commitment; attention to detail; demonstrated ability to work with deadlines and manage conflicting priorities; excellent communication skills; ability to work with highly qualified professionals with international backgrounds.

Summary of conditions:

- Full time work (37,5h/week)
- Contract Length: Temporary
- Location: Bellaterra (Barcelona)
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: as soon as possible

How to apply:

All applications must be made via the ICN2 website <https://jobs.icn2.cat/job-openings/610/postdoctoral-researcher-alcoat-first-principles-studies-of-the-protection-of-steel-against-corrosion-using-scrap-aluminium> and include the following:

1. A cover letter.
2. A full CV including contact details.
3. 2 Reference letters or referee contacts.

Deadline for applications: 19/04/2024

Equal opportunities:

ICN2 is an equal opportunity employer committed to diversity and inclusion of people with disabilities.

ICN2 is following the procedure for contract of people with disabilities according with article 59 of the Royal Decree 1/2015, of 30 of October.