

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 behavior of matter at the nanoscale. ICN2 has been awarded with the Severo Ochoa Center of Excellence distinction for two consecutive periods (2014-2018 and 2018-2022). ICN2 comprises 18 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 (Intersect Project)

Research area or group: Theory and Simulation

Description of Group/Project:

The Theory and Simulation Group develops efficient methods for atomistic simulations in nanostructured systems, which can fully exploit modern computer multiprocessor architectures, and applies them to selected problems in Nanoscience and Nanotechnology. These include (but are not restricted to) the SIESTA (see www.icmab.es/siesta) and TranSIESTA codes. SIESTA is a multi-purpose first-principles method and program, based on Density Functional Theory, which can be used to 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. Both codes are among the most important of their kind and are widely used by the academic community.

Main Tasks and responsibilities:

- Development of different new computational methods within the SIESTA package to extract physical properties, which might include: formation enthalpy of charged defects, electron-phonon matrix elements from linear response (DFPT), dissipation scattering rates for electrical and thermal conductivity, dynamics of domain walls in ferroic materials, or defect diffusion barriers.
- Implementation and testing of workflows for high-throughput calculations.
- Preparation of scientific reports, papers and software documentation.
- Attendance at project meetings, and scientific conferences, and participation in outreach activities within the project.
- Contribution to students' supervision.
- Contribution to other activities in the group.

Education, Experience, Knowledge and Competences required:

- Education
PhD in Physics, Materials Science, Chemistry, Computer Science, or related disciplines.
- Knowledge
DFT methods, coding in Fortran+MPI, python.
- Professional Experience
Experience in computational science (ideally, with SIESTA), high-performance computing, and high-throughput calculations.

- **Competences**

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

Research Career Profile (According to the European Framework for Research Careers):

R3 Established Researcher

Summary of conditions:

- Full time work (37,5h/week)
- Contract Length: 1 year renewable yearly until 3 years.
- 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 and include the following:

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

Equal opportunities:

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