

ICN2 is a renowned research centre. Its research lines focus on the newly discovered physical and chemical properties that arise from the behaviour of matter at the nanoscale.

The Institute promotes collaboration among scientists from diverse backgrounds (physics, chemistry, biology, and engineering) to develop basic and applied research, while seeking out new ways to interact with local and global industry.

It also offers researchers training in nanotechnology, develops numerous activities to promote and enable the uptake of nanotechnology by industry, and promotes networking among scientists, engineers, technicians, business people, society, and policy makers.

ICN2 was accredited in 2014 as a Severo Ochoa Centre of Excellence and is a founding member of the Barcelona Institute of Science and Technology (BIST). The aim of the Severo Ochoa Program, sponsored by the Spanish Ministry of Economy, Industry and Competitiveness, are to identify and support those Spanish research centres that demonstrate scientific leadership and impact at global level.

## **Job Title: Postdoctoral Researcher (MaX-CoE 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](http://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.

The positions are framed within the spirit of the SIESTA-project, with a close collaboration between teams at the ICN2 (Pablo Ordejon, Barcelona), the ICMAB (Alberto García, Barcelona), and CIC nanoGUNE (San Sebastian, in collaboration with Emilio Artacho, in Cambridge).

### **Main Tasks and responsibilities:**

The work focuses on using advanced programming tools to transition SIESTA, one of the MaX flagship codes, to exascale architectures, and enable its use for high-throughput calculations under the AiiDA infrastructure. Among the objectives of the position(s) within MaX-CoE we include:

- Modularising MAX codes to foster maintainability, to consolidate similar functionality within a single code and across different MAX codes and to enable the use of performance tuned and architecture adjusted modules.
- Utilising advanced programming schemes and methods to make the codes ready for heterogeneous pre-exascale architectures and to implement new algorithms.

- Enabling the use of MAX codes in high-throughput calculations, providing an additional avenue to leverage and saturate exascale performance.
- Implementation and testing of workflows for high-throughput calculations.
- Preparation of scientific reports, papers and software documentation.
- 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.
- Salary according to the cost of living in Barcelona.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: January 2019.

#### **How to apply:**

All applications must be made via the ICN2 website <http://jobs.icn2.cat/job-openings/160/postdoctoral-researcher-max-coe-project> 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: December 10.

#### **Equal opportunities:**

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