

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 20 Research Groups, 7 Technical Development and Support Units and Facilities, and 2 Research Platforms, covering different areas of nanoscience and nanotechnology.

**Job Title: Research Assistant**

**Research area or group:** Theory and Simulation Group

**Description of Group/Project:**

The Theory and Simulation Group has broad experience in the development of electronic structure methods and their application in order to perform atomistic simulations of molecules and materials. These include (but are not restricted to) SIESTA ([www.siesta-project.org](http://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 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. SIESTA is widely used by the academic community (about one thousand citations per year), and has been a flagship code of the MaX European Centre of Excellence for exascale computing in Materials Science ([www.max-centre.eu](http://www.max-centre.eu)) since its inception in 2015.

**Main Tasks and responsibilities:**

- Application of SIESTA and/or TranSIESTA to the study of materials at the nanoscale.
- Execution and analysis of SIESTA/TranSIESTA-based simulations in HPC facilities.
- Contribution to the development of new methodological approaches using SIESTA and/or TranSIESTA.
- Development and validation of SIESTA training materials.
- Contribution to SIESTA user training and to the organisation of SIESTA training events.
- Preparation of scientific reports, journal articles, posters, and oral presentations.
- Contribution to other activities in the group.

**Requirements:**

- **Education:**  
B.Sc. and M.Sc. in Physics, Materials Science, Chemistry, Computer Science, or related disciplines.  
M.Sc. must have been completed in 2022 or later.
- **Knowledge:** DFT-based methods.
- **Professional Experience:**  
Previous experience with SIESTA will be a plus but it is not essential.  
Previous experience with user-level High Performance Computing will be a plus but it is not essential.
- **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: 1 year
- Location: Bellaterra (Barcelona)
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: 1<sup>st</sup> October 2023

### 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.

Deadline for applications: 8 September 2023

### 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.