

As a flagship research center in nanoscience and nanotechnology, our mission is to open and explore new frontiers of knowledge at the nanoscale, and bring value to society in the form of new understanding, capabilities and innovation, while inspiring and providing broad training to the next generations of researchers. Our values are Commitment, Collaboration and Transformation.

Our 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

**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](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 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 use of shared research infrastructures in nanoscience and nanotechnology is facilitated under the EU-funded **NEP project**. The project provides free access to a wide portfolio of services to users and support excellence of science and technology while addressing complex nanoscience challenges. By expanding and consolidating the operation of an Interoperable Distributed Research Infrastructure for Nanoscience (IDRIN), the project supports research on materials and functional systems at the nanoscale and at the microscale.

Specifically, the work will be carried out at the Theory and Simulation Group at ICN2 <https://nffa.eu/offer/area/?id=6471>. **The Theory & Simulation Installation** is open to experimental users with no experience in modelling and simulation, as well as to experimental and computational users with experience in the field.

- Projects from experimental users are expected to request assistance on measurements performed either in combination with another NFFA installation or outside the NFFA facility. In the latter case the computational project should address recent experimental results on nanoscience and may lead to novel experiments.
- Projects from theory users are expected to request assistance on multi-scale/multi-physics simulations involving at least two independent computational methods (e.g. electronic ground-state and excited-state approaches, molecular dynamics and electronic structure, structural and spectroscopic properties ...).

### Main Tasks and responsibilities:

- Perform a bibliographic research on the topic of the NFFA access, contrasting experimental information with previous theoretical works in the literature.
- Contact the external user in case clarifications are needed.
- Design and execute the required atomistic simulations to extract the relevant information. These could involve electronic structure calculations (SIESTA/TranSIESTA), or Molecular Dynamics (including hybrid QM/MM or ML-IP simulations)
- Apply for computational resources in HPC facilities when needed.
- Prepare periodic reports of the results and provide feedback to experiments (when required)
- Write scientific manuscript for publication.

### 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, ML and/or MD codes.
  - 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.
- Work-Life Balance and Flexibility with flexible work schedules
- 28 holidays per year
- Flexible compensation plan: tax advantages contracting some products (health insurance, childcare, training, among others.)
- Training activities: languages, mentoring programme, wellbeing programme.
- International environment

Estimated Incorporation date: May 2025

**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: No deadline. Applications will be continuously reviewed.

**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.