

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**

### **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 since its inception in 2015.

The Theory and Simulation Group participates in HANAMI (HPC Alliance for Applications and Supercomputing Innovation: the Europe - Japan collaboration). HANAMI is three-year-long collaboration of 14 European research institutions and is funded (<https://cordis.europa.eu/project/id/101136269>) by the European High Performance Computing Joint Undertaking as part of the Horizon Europe program. HANAMI supports the development and the improvement of the performance and transferability of European and Japanese HPC applications by leveraging the skills and expertise of the scientific community within Europe and Japan.

The Theory and Simulation Group will contribute to HANAMI on the topic of first-principles electrochemistry and battery research. This will be done in close collaboration with the research group of Minoru Otani at the University of Tsukuba. The work will be based on the Effective Screening Medium (ESM), a method and software (<https://sugino.issp.u-tokyo.ac.jp/esm/>) for the study of electrified interfaces. ESM already has an interface for SIESTA, but at the moment it is not yet compatible with the most modern versions of SIESTA. The work will comprise the design and implementation of a new interface between ESM and the latest version of SIESTA, its validation, its benchmarking, and its exploitation in scientific applications. Work will also involve the optimization of SIESTA on the fastest and most powerful HPC infrastructures in Japan (FUGAKU,...).

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

The post holder will become the central person in the collaborative effort described above. Work will involve interfacing ESM with the most modern versions of the SIESTA code, as well as benchmarking and optimization of SIESTA (including the ESM module) on the most important HPC infrastructures in Japan. Additionally, once the codes have been tested and validated, the work will involve performing simulations of materials for energy storage (batteries, supercapacitors), in collaboration with our partners in Japan (Prof. Minoru Otani).

The post holder will undertake the following tasks:

- Contribution to the design, implementation, testing and demonstration of new methodologies and algorithms for the study of electrochemical processes.
- Performing benchmarks in HPC machines in Japan and carrying optimizations to improve performance of the codes.
- Execution of simulations in top HPC facilities, both in Europe and Japan.
- Contribution to the writing of applications to HPC centres (including EuroHPC systems) in order to secure the computational resources needed.
- Travel to Japan. It is expected that the post holder will visit the group in Tsukuba, Japan for about 1 month per year of employment. The post holder will contribute to the writing of HANAMI travel grant applications (HANAMI travel funds are held by the coordinating institution and they are allocated through recurrent internal calls).
- Preparation of scientific reports, journal articles and software documentation.

#### Requirements:

- **Education:**  
PhD in Physics, Materials Science, Chemistry, or related disciplines.
- **Knowledge and Professional Experience:**  
DFT-based methods.  
First-principles electronic structure calculations and user-level high performance computing.  
Programming skills: FORTRAN  
Ability to communicate effectively in English (English is the working language of the Theory and Simulation Group and of HANAMI).
- **Optional:**  
Previous experience with first-principles electrochemical simulations.  
Previous experience with SIESTA / TranSIESTA.  
Previous experience with ESM.  
Familiarity with RIKEN HPC systems and/or other Japanese HPC facilities.  
Familiarity with EuroHPC HPC systems.  
Ability to read Japanese.  
Experience in parallel scientific programming.  
Experience with High Throughput calculations.  
Other research and software engineering experience will be considered
- **Personal Competences:**  
Availability to travel to Japan for one month per year of employment.  
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 background.

#### Summary of conditions:

- Full time work (37,5h/week)
- Contract Length: Temporary (2 years)
- 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/621/postdoctoral-researcher-hanami-theory-and-simulation-group> 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. 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.