

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 17 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

Description of Group/Project:

The Theory & Simulations group has broad experience in development and applications of electronic structure tools, including advanced workflows for atomistic modelling in nanoscience. The group is core developer of the SIESTA ab initio method, a flagship code of the MaX European Centre of Excellence for exascale computing in Materials Science (www.max-centre.eu). Within MAGNIFIC we will theoretically explore the interplay between electron, phonons and photons in nanocrystalline silicon for nano-opto-electro-mechanical devices. Interatomic potentials based on ML will be used to build realistic atomistic structures of the grain boundaries in nc-Si, and to study their vibrational (thermal) properties. DFT calculations will be used to characterize the electronic properties and build Effective Hamiltonian models. Methods to incorporate the reciprocal interactions between electrons and phonons at simple grain boundaries from first principles will be explored and developed.

Main Tasks and responsibilities:

1) Implement reliable ML interatomic potentials (MLP) based on DFT calculations for nanocrystalline silicon (grain boundaries and AlN interfaces); 2) building effective Hamiltonian models for the electronic properties of the materials; 3) extract electronic and thermal transport properties from dynamical simulations; 4) prepare scientific documentation, articles and reports; 5) participate in the collaboration with the experimental partners in the project; 6) contribute to other activities in the group.

Requirements:

- **Education**
PhD in Physics, Materials Science, Chemistry, or related disciplines
- **Knowledge**
Knowledge of DFT methods (ideally with SIESTA, but not essential)
- **Professional Experience**
Professional experience in computational science, high-performance computing and high-throughput calculations; Fortran+MPI, python and/or other programming languages
- **Personal Competences**
Demonstrated ability to work with deadlines, manage conflicting priorities; excellent communication skills; strong commitment, attention to detail and ability to work with highly qualified professionals with international backgrounds.

Research Career Profile (According to the European Framework for Research Careers): R2

Summary of conditions:

- Full time work (37,5h/week)
- Contract Length: 2 years.
- Location: Bellaterra (Barcelona)
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: January 2023

How to apply:

All applications must be made via the ICN2 website <https://jobs.icn2.cat/job-openings/447/postdoctoral-researcher-magnific-project-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.