

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: THERMOS software developer**

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

**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](http://www.max-centre.eu)). THERMOS aims to bring academic codes for the simulation of thermal transport to a new level, transforming them into industry-grade simulation software which can be adopted in the industrial environment.

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

- 1) Implement software tools and workflows to adapt SIESTA and the thermal transport codes in use in the group to an industrial environment, within the ASAP simulation package developed by SIMUNE Atomistics SL
- 2) prepare documentation and reports
- 3) participate in the collaboration with other partners in the project
- 4) contribute to other activities in the group.

### **Requirements:**

- **Education:**  
Bachelor or PhD degree in Computer Science, Physics, Materials Science, Chemistry, or related disciplines
- **Knowledge and Professional Experience:**  
Experience in computational science and frameworks for high-throughput calculations  
Competence in Python scripting is a requisite.  
Fortran knowledge will be very highly valued, and 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.

### **Summary of conditions:**

- Full time work (37,5h/week)
- Contract Length: Temporary (1 year)
- 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/561/thermos-software-developer-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.

Applications will be continuously reviewed. Shortlisted candidates will be invited for interview.

**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.