



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 the Severo Ochoa Center of Excellence distinction for two consecutive periods (2014-2018 and 2018-2022). ICN2 comprises 18 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: modelling of thermal transport in layered material systems

**Research area or group:** "Theory and Simulation" and "Ultrafast Dynamics in Nanoscale Systems"

## **Description of Group/Project**:

We have an opening for a highly motivated postdoctoral researcher to work on an interdisciplinary theoretical-experimental project that aims at understanding and controlling thermal transport properties in atomically thin layered materials, with relevance for applications such as thermoelectrics and thermal management. The position is linked with the European project INTERSECT and the Spanish project STEAMY. The successful candidate will be part of both the "Theory and Simulation" group (led by Pablo Ordejón) and the "Ultrafast Dynamics in Nanoscale Systems" group (led by Klaas-Jan Tielrooij) at ICN2, and will benefit from the strong collaboration with the team of Associate Professor Zeila Zanolli, at the Condensed Matter and Interfaces Group at the Debye Institute for Nanomaterials Science in Utrecht (NL).

#### Main Tasks and responsibilities:

- Develop numerical tools (codes and workflows) to calculate thermal properties of materials from Density Functional Theory calculations
- Perform simulations to compute semi-classic transport coefficients from first-principles electronic structure
- Design experiments based on simulations results
- Perform simulations to interpret experimental results obtained with state-of-the-art ultrafast techniques

#### Education, Experience, Knowledge and Competences required:

- Education
  - PhD in Physics, Chemistry, Materials Science or related disciplines.
- Professional Experience
  - Experience with modelling of thermal transport properties with BoltzTrap Experience in use of first-principles (DFT) codes to predict electronic properties at the nanoscale Experience in high-throughput simulations and data management Experience in Fortran and Python programming Experience with layered materials is a bonus
- Competences

Strong commitment, excellent communication skills, ability to work with highly qualified professionals with international backgrounds, taking responsibilities, independence.





## Summary of conditions:

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

Estimated Incorporation date: October 2020

## How to apply:

All applications must be made via the ICN2 website <u>https://jobs.icn2.cat/job-openings/240/postdoctoral-researcher-modelling-of-thermal-transport-in-layered-material-systems</u> 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: July 31st 2020.

## Equal opportunities:

ICN2 is an equal opportunity employer committed to diversity and inclusion of people with disabilities.