

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 20 Research Groups, 7 Technical Development and Support Units and Facilities, and 2 Research Platforms, covering different areas of nanoscience and nanotechnology.

### **Job Title: PhD Student**

**Research area or group:** Theoretical and Computational Nanoscience Group

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

The TCN group is launching an activity on marrying Artificial Intelligence with its activities and numerical tools to access charge transport information in complex (disordered) van der Waals heterostructures. The project will contribute to the establishment of such a platform and interface with in-house computational artillery of TCN ([www.lsquant.org](http://www.lsquant.org)) and to demonstrate predictive power of the methodology on neuromorphic computing applications.

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

- Perform DFT simulations on 2D materials such as transition metal dichalcogenides.
- Develop machine learning potentials and molecular dynamics simulations.
- Contribute to the implementation of developed tools on the in-house LSQUANT code ([www.lsquant.org](http://www.lsquant.org)) and computing architecture of TCN/ICN2

### **Requirements:**

- **Education:** PhD in physics or electrical/ mechanical engineering
- **Knowledge:** quantum mechanics, DFT simulations, programming machine learning techniques.
- **Professional Experience:** Programming in PYTHON/C languages
- **Personal Competences:** Demonstrated competitive ability in using DFT simulations, and machine learning techniques (optional)

### **Summary of conditions:**

- Full time work (37,5h/week)
- Contract Length: Temporary (4 years)
- Location: Bellaterra (Barcelona)
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.

Estimated Incorporation date: during early 2024

**How to apply:**

All applications must be made via the ICN2 website <https://jobs.icn2.cat/job-openings/549/phd-student-theoretical-and-computational-nanoscience-group> 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: 30/10/23

Applications will be evaluated as they are received.

El contrato es parte de la ayuda PID2022-138283NB-I00, financiado por MCIN/AEI/10.13039/501100011033 y por el FSE+ invierte en tu futuro



**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.