As a flagship research center in nanoscience and nanotechnology, our mission is to open and explore new frontiers of knowledge at the nanoscale, and bring value to society in the form of new understanding, capabilities and innovation, while inspiring and providing broad training to the next generations of researchers. Our values are Commitment, Collaboration and Transformation.

Our 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: Research Assistant in Active learning

Research area or group: Theoretical and Computational Nanoscience Group

Description of Group/Project: In this short-term project we shall use active learning to accelerate the training of deep learning algorithms for optimising 2D material van der Waals (vdW) structure discovery. The goal is to make model training more data-efficient and to speed up candidate selection.

Main Tasks and responsibilities:
Core duty 1: The person shall deploy and interconnect an active learning framework into our simulation pipeline (data adapters, query strategy, retraining loop).

Core duty 2: The person shall perform benchmarks and tests to evaluate its efficiency, comparing active learning against simple baselines (e.g., random sampling).

Implement and compare basic acquisition strategies (e.g., uncertainty sampling, simple committee methods).

Define and track metrics (accuracy, label efficiency, convergence speed, runtime).

Keep experiments reproducible (scripts, configs, logs) and write a short technical report.

Requirements:

Minimum required:

- Enrolled BSc (Year 3–4) in Physics, Materials Science, Computer Science, or similar.
- Solid Python; basic PyTorch or TensorFlow.
- Intro ML knowledge (train/val/test splits, losses, overfitting).
- Comfortable with Linux and git.

The following features will be valued:

- Interest in active learning and/or uncertainty estimation.
- Curiosity about 2D materials and vdW heterostructures.

What You'll Learn:

- Practical active learning loops and acquisition strategies.
- How to integrate ML with a real materials simulation pipeline.
- Benchmarking, ablation studies, and reproducible research practices.

Deliverables:

- A working active learning module integrated with the pipeline.
- A concise benchmark report (figures/tables + short narrative).
- Clean code repository with a minimal example.

Summary of conditions:

- Part-time work
- Contract Length: 6 months

- Location: Bellaterra (Barcelona)
- Salary will depend on qualifications and demonstrated experience.
- Support to the relocation issues.
- Life Insurance.
- Work-Life Balance and Flexibility with flexible work schedules
- 28 holidays per year
- Flexible compensation plan: tax advantages contracting some products (health insurance, childcare, training, among others.)
- Training activities: languages, mentoring programme, wellbeing programme.
- International environment

Estimated Incorporation date: December 2025

How to apply:
All applications must be made via the ICN2 website 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: 02/10/2025

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.