



ICN2 is a renowned research centre. Its research lines focus on the newly discovered physical and chemical properties that arise from the fascinating behaviour of matter at the nanoscale.

We are looking for a suitable and highly motivated candidate to carry out the:

The icn2 groups involved are:

Student's tasks:

The Institute promotes collaboration among scientists from diverse backgrounds (physics, chemistry, biology, and engineering) to develop basic and applied research, always seeking interactions with local and global industry. ICN2 also trains researchers in nanotechnology, develops numerous activities to facilitate the uptake of nanotechnology by industry, and promotes networking among scientists, engineers, technicians, business people, society, and policy makers.

ICN2 was accredited in 2014 as a Severo Ochoa Centre of Excellence.

The Severo Ochoa Program, sponsored by the Spanish Ministry of Economy and Competitiveness, aims to identify and support Spanish research centres that are among the world's best in their specialty. This award is the highest recognition of centres of excellence in Spain, and it is granted after international scientific committees carry out a rigorous evaluation of project proposals submitted by Spanish research centres.

SEVERO OCHOA PhD ON NEW METHODOLOGIES FOR MODELLING VIBRATIONAL AND THERMAL PROPERTIES IN NANOMATERIALS AND NANODEVICES
Ref: 09-SO

- [Theory and Simulation](#)
- [Theoretical & Computational Nanoscience](#)
- [Phononic and Photonic Nanostructures](#)
- [Oxide Nanoelectronics](#)

The student's tasks will include:

- Develop and implement algorithms for efficient calculations of vibrational properties from first principles using Density Functional Perturbation Theory (DFPT) within the SIESTA package.
- Apply the new algorithms to compute phonon spectra and phonon-phonon coupling strengths in nanostructured systems.
- Perform simulations of thermal transport in low-dimensional nanostructures using the information derived from the vibrational properties.
- Adapt the DFPT methodology implemented to the calculation of properties related to the response to lattice deformations, aiming at simulations of piezo- and flexo-electric responses.



Profile of the candidate:

BSc in Physics, Chemistry, Materials Science or Nanoscience. Master degree with experience in materials simulations and (ideally) in numerical methods. Knowledge of linux/unix and programming experience (fortran and mpi) preferable. Good written and oral communication skills in English.

Skills to be acquired:

Expertise in first principles of atomistic simulations. Algorithm development and programming skills. Knowledge of vibrational properties in materials and thermal transport. Novel materials. Materials engineering and nanostructured bi-dimensional materials.

We offer:

- Full-time contract as a PhD researcher, for up to 3 years, extended yearly upon evaluation.
- Social benefits: Flexible timetable, Flexible Benefits Package
- Scientific excellence, a challenging project, and an innovative work environment.

How to apply:

Contact us through the online application form at :

www.jobs.icn2.cat/openings/9/severo-ochoa-programme-phd-fellowships/

Closing date:

Interested candidates are encouraged to apply by 31st August 2014. The recruitment process will be closed when a suitable candidate is found. Once the process is closed the announcement will no longer be available on the ICN2 jobs and fellowships site (www.jobs.icn2.cat).