

Doctoral Training Programme in Functional Advanced Materials (DOC-FAM)

DocFam+ (DOctoral training programme in Functional Advanced Materials: Towards a Better Future) is a new doctoral programme for the recruitment of 26 excellent doctoral researchers led by the Institute of Materials Science of Barcelona (ICMAB-CSIC).

DocFam+ is a unique interdisciplinary and intersectorial research programme. We offer excellent salaries and international experience through secondments. The complete training programme includes annual workshops, a career development retreat and industry days, among others.

More information: <https://docfam.icmab.es/>

Job Title: PhD Student - Multiscale modeling of electronic, spin and thermal transport in nanostructured materials

Description of the project/group:

Modeling transport in nanostructured materials is a challenging endeavor, due to the complexity of the physical processes and the multiple length and time scales involved. Transport of electrons, spins and heat (in the form of lattice vibrations) can now be studied from first principles (in particular, using Density Functional Theory), dealing with the full quantum-mechanical nature of these degrees of freedom. However, this can only be done for systems with a small number of atoms, far from those needed to address real devices. This project will address this issue, to develop theoretical and computational tools to bridge the atomistic description provided by first-principles methods to the meso and microscopic scales. Work will be done at ICN2, in the group of Prof. Pablo Ordejón (Theory and Simulation), in strong collaboration with other groups both at ICN2 (Stephan Roche on theory, Klaas Tielrooij on experiments), and abroad (David Broido at Boston College, and others).

Principal responsibilities:

The post holder will undertake the following tasks:

- Simulation of materials at the nanoscale using SIESTA/TranSIESTA
- Execution and analysis of SIESTA/TranSIESTA-based simulations in HPC facilities.
- Contribution to the development of new methodological approaches using SIESTA and/or TranSIESTA.
- Development and validation of SIESTA training materials.
- Contribution to SIESTA user training and to the organisation of SIESTA training events.
- Preparation of scientific reports, journal articles, posters, and oral presentations.
- Contribution to other activities in the group.

Education:

- B.Sc. and M.Sc. in Physics, Materials Science, Chemistry, Computer Science, or related disciplines.

Knowledge:

- DFT-based methods.

Experience:

- Previous experience with SIESTA will be a plus but it is not essential.
- Previous experience with user-level High Performance Computing will be a plus but it is not essential.

Competences:

Strong commitment; attention to detail; demonstrated ability to work with deadlines and manage conflicting priorities; excellent communication skills; ability to work with highly qualified professionals with international backgrounds.

More information and link to apply: <https://docfam.icmab.es/>