Postdoctoral Fellowship under the Marie S. Curie Actions Cofund project "Opening Sphere UAB-CEI to Postdoctoral Fellows (P-Sphere)" Gran Agreement 665919.

Department or Institution involved

Atomistic Simulations in Nanoscience

Topic description

The broad objective of the project is to advance in the ability to predict and explain the behavior of nanoscale systems, using theory and simulation methods and tools. This has two intertwined components. The first one is the development of theoretical methods and computational algorithms for atomistic simulations in nanoscale systems, including the implementation of these in computer codes that become a reference and basic research tool for other research groups worldwide. The second one is their application to particular problems in Nanoscience and Nanotechnology, with a very special focus on the direct collaboration with experimental groups. Within the activities related to methodological developments, the researcher will join one of the founding and leading developers of SIESTA and TranSIESTA. SIESTA is a multi-purpose first-principles method and code, based on Density Functional Theory, which can be used to describe the atomic and electronic properties of systems, currently with up to several thousands of atoms (therefore, falling right in the nanoscale regime). TranSIESTA is an extension of SIESTA that enables the study of electronic transport phenomena in nanoscale devices. Both codes are among the most important and most widely used by the academic community, with more than 4,000 registered users worldwide, and the articles describing these methodologies have gathered so far more than 10,000 citations.

The candidate will perform theoretical simulations in support to experimental research, in topics that include (but are not limited to): Energy harvesting (photovoltaic, photochemistry, electromechanical membranes, etc), energy efficiency (thermal dissipation), and future spintronics devices.

Project supervisor & hosting group

Prof. Pablo Ordejon is director of ICN2 and Leader of the Theory and Simulation Group. He is author of around 190 publications in international peer-reviewed scientific journals (~19,000 citations, h-index = 50; source: Web of Science, Jun. 2015). Expert in electronic structure methods for the study of systems with large number of atoms, and one of the pioneers in the development and application of the so-called Order-N methods (which scale linearly with system size, thus allowing tackling systems with an unprecedented number of atoms). He has also pioneered the combination of Density Functional Theory and Non-Equilibrium Greens Functions methods for the simulation of electronic transport phenomena in nanoscale devices from first-principles. He is one of the three Founding Members of the team that develops the SIESTA code. In the last ten years, he has had an intense activity of service to the research

community, being Editor in several international journals (EPL and Physica Status Solidi, currently), Responsible for the Condensed Matter Physics Area of the Spanish National Scientific Evaluation Agency (ANEP), and Coordinator of the Physics and Engineering Access Panel of the Barcelona Supercomputing Centre (BSC) and the Spanish Supercomputing Network (Red Española de Supercomputación - RES).

Prof. Pablo Ordejón is the Director of the "Severo Ochoa Centre of Excellence Award", a competitive Grant from Spanish MINECO (Ministry of Economy and Competitiveness), which has been awarded to ICN2 in 2014, and is focused on "Nanodevices for Social Challenges".

The group also participates in two recently funded European projects:

- "NFFA: Nanoscience Foundries and Fine Analysis for Europe", focused in implementing the first integrated, distributed research infrastructure as a platform supporting comprehensive user projects for multidisciplinary research at the nanoscale, extending from synthesis and nano lithography to nanocharacterisation, theoretical modelling and numerical simulations, through a coordinated open-access to complementary facilities.
- "MaX: Materials design at the eXascale", a Center of Excellence that supports the efforts of the community of European teams working in open-source codes for materials modelling, simulations, and design, in close collaboration with HPC facilities and industrial and academic stakeholders as final users of the computational tools.

Candidate's profile

A PhD in physics, chemistry, or materials science. The ideal candidate will have prior experience in first principles atomistic simulations (DFT calculations), and interest in theory and simulation of condensed matter, low dimensional systems and nanostructures, and programming skills (preferably in fortran/mpi). She/he should have good written and oral communication skills in English, be a good team player, creative and have the ability to work independently.

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