Call reference number	(2026-34)
Call name	Predoctoral researcher position on magnetotransport in nanostructured materials
Application Deadline	2027/01/31

Introduction and main description

How does a network of nanoscale building blocks conduct electricity in a magnetic field? And how does its response change when the network deforms?

BCMaterials, Basque Center on Materials, Applications and Nanostructures, Leioa, Spain, invites applications for a predoctoral researcher position in computational materials science. The main project will investigate magnetotransport in nanostructured materials, from representative nanoscale components and junctions to complex networks, using a multiscale approach that connects atomistic and continuum descriptions. A complementary research direction will focus on perovskite-based heterostructures and their interfaces with nanocarbons and other low-dimensional materials for sustainable energy applications.

The researcher will be jointly supervised by Dr Karolina Z. Milowska, Ikerbasque Research Fellow and Ramón y Cajal Fellow, and Dr Sergio Lucarini, Ikerbasque Research Fellow and Ramón y Cajal Fellow, both at BCMaterials. The project will combine atomistic and quantum-transport modelling with continuum mechanics and multiphysics simulations. A significant part of the work will involve scientific programming and the development and adaptation of computational tools and workflows.

The main research direction will focus on understanding how the electronic transport of nanostructured materials changes under magnetic field and deformation. The work will progress from representative building blocks, bundles and junctions towards increasingly complex systems and network-level descriptions. The researcher will also contribute to modelling hybrid halide perovskites interfaced with nanocarbons and other two-dimensional materials, with the aim of understanding and designing interfaces relevant to sustainable energy technologies.

The position is particularly suited to a candidate who enjoys working across multiple scientific problems, learning new computational methods and collaborating closely with both theoreticians and experimental researchers. The successful candidate will join an interdisciplinary research environment at BCMaterials and will have opportunities to contribute to publications, conference presentations and international collaborations.

This is a full-time position. The successful candidate will be employed on an initial one-year contract. An extension is expected, subject to satisfactory progress. Competitive salary and benefits will be offered.

Skills and Requirements

We are looking for an person with a strong interest in computational materials research and enthusiasm for working at the interface of condensed-matter physics, quantum chemistry and materials science. The ideal candidate should have previous experience in theoretical or

Skills and Requirements

modelling-based research, for example gained during a Master's project, and a strong background in physics and mathematics. A good knowledge of quantum mechanics is expected. The candidate needs to hold an MSc or equivalent degree in Physics, Mathematics, Chemistry or a closely related field by the starting date. Practical programming experience in Python and knowledge of or experience with at least one computational method used to study materials or nanoscale systems, such as density-functional theory (DFT), tight-binding (TB), density-functional tight-binding (DFTB) or molecular dynamics (MD), are required.

Good communication, analytical and problem-solving skills, as well as a self-driven approach to learning, are fundamental. The candidate must be able to work both independently and as part of a research team, including in close collaboration with experimental researchers. As the researcher will contribute to more than one research direction, the ability to organise their work effectively, manage parallel research tasks and adapt to different scientific problems is also essential. Proficiency in written and spoken English is mandatory.

Experience with more than one of the computational methods listed above, knowledge of Fortran and/or C++, or previous use of SIESTA, QuantumATK, MATLAB, Mathematica, Maple or COMSOL will be additional assets. Previous experience in quantum transport, continuum mechanics or multiscale modelling will also be beneficial. We will particularly value evidence that the candidate has successfully worked on more than one project or across different research areas, for example through Master's research, internships or collaborative projects. These additional qualifications are not obligatory, but they will strengthen the application and will be taken into account during candidate selection.

Work Program / Duties / Responsibilities

Magnetotransport: from representative components to complex networks
The main research will examine how magnetic fields influence electrical transport in networks assembled from low-dimensional materials. Starting from representative building blocks, bundles and junctions, the work will progress towards increasingly complex architectures and network-level descriptions. Particular attention will be paid to how local atomic structure, interfacial coupling, quantum interference, temperature and deformation influence the collective electrical response.

The multiscale component will connect atomistic transport calculations with continuum and micromechanical models. It will explore the coupling between magnetotransport and magnetomechanical behaviour, including how deformation and field-driven microstructural rearrangements in magnetically responsive systems modify junction geometries and conducting pathways. The aim is to distinguish direct magnetic-field effects on electronic transport from changes mediated by the evolving structure.

Complementary research: perovskite interfaces for sustainable energy
The researcher will also contribute to atomistic studies of hybrid halide perovskites interfaced with nanocarbons and other two-dimensional materials. This work will investigate how interfacial structure and chemical interactions affect electronic states, charge redistribution and structural stability, guiding the design of heterostructures for sustainable energy generation in close collaboration with experimental researchers at BCMaterials.

Work Program / Duties / Responsibilities
Duties and Responsabilities Developing, extending, testing and documenting simulation codes and numerical workflows will be an important part of the position. The work will combine electronic-structure and molecular-dynamics calculations with tight-binding quantum transport based on non-equilibrium Green's functions and continuum modelling. The researcher will analyse and interpret results, contribute to publications and presentations, and work closely with theoretical and experimental collaborators. Contributions to the main and complementary research strands will be planned jointly with the supervisors.

Application Procedure
Apply by submitting a motivation letter and a CV (in English), besides a recommendation letter and/or a list of referees (if possible), using the "Contact" button at the corresponding offer, at the "Join Us" area on BCMaterials' portal (https://www.bcmaterials.net/join-us). Your name and email address will be required for furher contact too.

Other Relevant Information
The position offers joint supervision across atomistic and continuum approaches, training in computational materials research and scientific software development, and close interaction with experimentalists at BCMaterials and international collaborators. The researcher will address fundamental physical questions while contributing to the design and understanding of materials for practical applications. We provide a highly stimulating environment with state-of-the-art infrastructures, and unique professional career development opportunities. We offer and promote a diverse and inclusive environment and welcome applicants regardless of age, disability, gender, nationality, ethnicity, religion, sexual orientation or gender identity.