

<b>Call reference number</b>	(2023-05)
<b>Call name</b>	Pre-doctoral IKUR positions: Computational Materials Science
<b>Application Deadline</b>	2023/02/05

### Introduction and main description

BCMaterials, Basque Center on Materials, Applications and Nanostructures, Leioa, Spain ([www.bcmaterials.net](http://www.bcmaterials.net)), is an autonomous research center, belonging to Ikerbasque, the Basque Foundation for Science and the University of the Basque Country (UPV/EHU). IKUR is the strategic program promoted by the Education Department of the Basque Government to boost Scientific Research in specific strategical areas, including Quantum Technologies, High Performance Computing, Neutronics and NeuroBiosciences.

We are seeking a highly motivated PhD student to join the MonteQarlo research project funded by the IKUR program. MonteQarlo focused on the development of quantum algorithms for molecular simulations. The successful candidate will be working on adapting the Markov-chain Monte Carlo method and the Virtual move Parallel Tempering algorithm to be run on gate model and quantum annealing quantum computers. This project will involve collaboration with industry partners and the opportunity to work with state-of-the-art quantum computers.

The ideal candidate will have a strong background in physics, computer science, or a related field, and experience in computational modeling and algorithms is desirable. Familiarity with quantum computing and molecular simulations is a plus, but not required. The candidate should have excellent problem-solving skills and the ability to work independently as well as in a team.

This is a full-time position and the successful candidate will be enrolled in a PhD program at UPV/EHU. The position is funded for 3 years.

The work will be carried out at BCMaterials in the Computational Soft Matter and Biophysics group and in close collaboration and coordination with different institutions from the Basque Scientific and Technological network as well as in cooperation with international leading research institutions. In particular, the other parttern of the MonteQarlo project is the Intelligent Systems Group under the supervision of Dr José Antonio Pascual Saíz and Dr Javier Navaridas Palma at the UPV/EHU.

For the successful candidate, the position represents an excellent opportunity to develop both collaborative and personal scientific research career, exploiting the capabilities of advanced functional materials and their application.

### Skills and Requirements

The candidate must have a Master in Materials Science, Chemistry, Physics, Biology, Biotechnology or related areas.  
 Proficiency in speaking and writing in English.

### Skills and Requirements

Self-motivated and ability to work in a team and willing to coordinate the research in a particular topic.

A high level of motivation and independent thinking abilities.

Ability and eagerness to learn new skills outside own discipline

Presentation skills and able to meet the deadline are also required.

### Work Program / Duties / Responsibilities

The PhD candidate will work in an ambitious research program in one of the aforementioned research areas. Materials will be designed, characterized, the functional properties evaluated and optimized and their integration into applications demonstrated, whenever suitable.

The main activity of the successful candidate will be to combine the computational power of Quantum Computing with the advantages offered by the Virtual Move Parallel Tempering (VMPT) algorithm. We will then test our approach to the study of protein folding and protein design. The frustration coming from the heterogeneous interaction between the amino acids make both problems computationally hard, hence they are an ideal test system to test the efficiency of our new quantum VMPT

### Application Procedure

Apply by submitting a motivation letter and a CV (in English) 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 further contact too.

### Other Relevant Information

Include contact details for 2 referees.

Interview will be conducted soon after the deadline.

The preferred starting date to join is February 2022.