

Call reference number	(2023-04)
Call name	Post-doctoral IKUR positions: Computational Materials Science - Automation drug Screening
Application Deadline	2023/02/05

Introduction and main description

BCMaterials, Basque Center on Materials, Applications and Nanostructures, Leioa, Spain (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 and qualified individual to join the ReUSED project "Ultra-wide Screening of anti-viral Drugs" team as a research scientist funded by the IKUR program. The ReUSED project aims to apply recent technological advances in computational modeling and graphene-based devices to develop a novel method for automating drug screening. The successful candidate will work on combining large-scale computational screening with fast experimental testing using printed graphene field effect transistors (gFETs). The focus of the project will be on developing new antiviral drugs, with the ultimate goal of quickly identifying and distributing effective treatments in the event of a viral outbreak.

This is a full-time position based at our research facility in the Basque region. The duration of the contract is estimated in two years, until the end of the project. We offer a competitive salary and benefits package, as well as the opportunity to work on an exciting and meaningful project with the potential to have a significant impact on global health.

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 partners of the ReUSED are the groups of Prof Maurizio Prato at CIC biomAGUNE, Prof Jose Luis Vilas at the UPV/EHU and of Prof Senentxu Lanceros-Méndez at BCMaterials.

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

PhD in Materials Science, Chemistry, Physics, Biology, Biotechnology or related areas.
 A strong background in computational modeling and/or graphene-based devices.
 Experience with microfluidics and drug screening techniques is also highly desirable.
 Proficiency in speaking and writing in English.
 Self-motivated and ability to work in a team and willing to coordinate the research in a

Skills and Requirements

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 tasks associated to this position are:

Task 1.1 Drug Docking

ReUSED will apply the Drug Docking approaches to score the binding the FDA approved drugs to the structure of the target viral proteins predicted within the Machine Learning methods (e.g., AlphaFold).

Task 1.2 Protein Structure and binding modelling

Protein structure prediction methods in the last few years made a giant leap forward and are now capable of reliably predicting the structure of complex proteins just from the knowledge of their genetic makeup.

The responsibilities of this position include:

- Design and execution of computational and experimental studies.
- Participating in experiments using gFETs to identify ligands that can block the binding of viral proteins to receptors.
- Collaborating with team members in the manufacturing of printed gFETs and the microfluidic system needed for automation.
- Analyzing and interpreting data, and preparing reports and presentations on research findings.
- Contributing to the writing of scientific papers and grant proposals.

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.