Call reference number	(2023-08)
Call name	Pre-doctoral IKUR position: Computational Nanochemistry
Application Deadline	2023/02/05

Introduction and main description

Maximum 1.000 characters for introduction and 3.000 for main descriptionBCMaterials, 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 Perfor-mance Computing, NeutrIonics and NeuroBiosciences.

We are seeking a pre-doctoral student to join our research team in the framework of the Graal project titled "Developing an Adaptive Machine Learning Platform for Computational Chemistry" funded by the IKUR program. The overall goal of this project is to create a fully automated platform that utilizes machine learning methods to train a variety of molecular properties for use in computational chemistry simulations.

The student will focus on the accurate description of colloidal quantum dots (QDs), an emerging material with outstanding optoelectronic properties that can be employed in electroluminescent displays, automated driving, etc. The idea is to employ machine learning tools to accelerate molecular dynamic simulations in a timescale (nanoseconds) to study processes in direct competition with light emission of these materials and thus to find ways to drastically improve the performance of these materials.

The work will be carried out at BCMaterials in close collaboration and coordination with different insti-tutions from the Basque Scientific and Technological network as well as in cooperation with interna-tional leading research institutions.

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. Competitive salary and benefits will be offered. If you are interested in this opportunity, please submit a CV and cover letter outlining your relevant experience and research interests.

Skills and Requirements

The candidate must have a Master in Materials Science, Chemistry, Physics, Biology, Biotechnology or related areas.
A strong background in computational chemistry and machine learning is desirable but not compulsory.
Proficiency in speaking and writing in English.
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.

Skills and Requirements
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 make use of the proposed automated platform to train with machine learning methods, forces and electronic structure properties of quantum dots, in particular III-V materials such as InP and InAs, on a subset of geometrical structures computed at the density functional theory level (DFT). Subsequently, the predoc will use machine-learning algorithms to predict quantum dot energy and forces at a fraction of the DFT time but with the same accuracy. This will allow to propagate the molecular dynamics simulations to timescales not attained before with DFT, specifically for these larger systems. The successful candidate will be expected to contribute to the development and implementation of this platform. They will also be responsible for conducting independent research and contributing to the publication of research findings. The PhD student will be incorporated at BCMaterials at the Computational Materials Science transverse lines under the supervision of Ivan Infante and Ivan Coluzza, Ikerbasque Research Professors. The PhD student will also have two co-supervisors, one at the DIPC with Ignacio Arganda-Carreras and one at the Vrije Universiteit Amsterdam with Lucas Visscher. In both these institutes the student will perform secondments.

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 furher 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.