

Company 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 strategic areas, including Quantum Technologies, High Performance Computing, Neutronics 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

Information

 Deadline: 2023-02-05
 Category: Academia
 Province: Bizkaia

 Country: Basque Country
 City: Leioa

Company

BCMaterials



Main functions, requisites & benefits

Main functions

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.

Requisites

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. Ability and eagerness to learn new skills outside own discipline. Presentation skills and able to meet the deadline are also required.