Call reference number	(2023-07)
Call name	Pre-doctoral IKUR position: Computational Soft Matter and Biophysics
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, NeutrIonics and NeuroBiosciences.

We are seeking a PhD student to join our research team in the project Graal titled "Developing an Adaptive Machine Learning Platform for Computational Chemistry" funded by the IKUR program. The 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 integration of Graal determined interaction of natural amino acids with water and polymeric based materials into the protein coarse-grained model "Caterpillar" developed with the Computational Soft-matter and biophysics group. The overall objective is to generate a new implicit solvent protein model capable of describing the interplay between folding and protein-polymer interactions.

The work will be carried out at BCMaterials 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.

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 compusolry.
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.

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 the interaction of amino acids with water and synthetic polymers such as PEG: 1) Building dataset with ab-initio molecular dynamic trajectories frames of amino acids in water with PEG 2) Combine ML potentials combined with protein coarse-grained model. 2) Production run of Monte Carlo simulation of the hybrid ML-coarse grained protein system. 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 Coluzza and Ivan Infante, Ikerbasque Research Professors. The PhD student will also have two co-supervisors, one at the DIPC with Ignacio Arganda-Carreras and one at the University of Vienna with Christoph Dellago. 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.