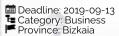


## POSTDOCTORAL FELLOWSHIP IN MACHINE LEARNING DRIVEN ATOMISTIC SIMULATIONS FOR

# Company Description

The Basque Center for Applied Mathematics - BCAM is an international research centre in the field of Applied Mathematics that was founded in 2008 by the Basque Government, the UVP/EHU and Ikerbasque. It also has the support of the Provincial Council of Bizkaia and Innobasque. It has a staff of more than 90 researchers of 25 nationalities working in various areas, from data science to mathematical modelling. and has twice been accredited as a centre of excellence "Severo Ochoa" by the State Research Agency, a distinction awarded to the best research institutions in the world in their field. www.bcamath.org

## Information



S Country: Basque Country ■ City: Bilbao Company BCAM



## Main functions, requisites & benefits

#### Main functions

The project "Machine-Learning-Driven Atomistic Simulations for Energy and Biomedical Applications" will be led by the group of Modelling and Simulation in Life and Material Sciences at BCAM (Basque Country) and the MS2Discovery Interdisciplinary Research Institute at Wilfrid Laurier University (Waterloo, Canada). Both groups are involved in the International Consortium on Multiscale Modelling of Advanced Energy Materials and collaborate extensively with physicists, mathematicians, theoretical/experimental chemists and engineers from a number of institutions around the world. The objective of the aforementioned project is to enable efficient and tractable simulations of several important classes of complex atomistic systems through the use of novel Machine Learning (ML) techniques, paying particular attention to those cases where state of the art Molecular Dynamics (MD) algorithms are lagging behind the current needs of challenging applications in energy and health. More info: http://www.bcamath.org/en/research/job/postdoctoral-fellowship-in-machine-learning-driven-atomistic-simulations-for-energy

### Requisites

Applicants must have their PhD preferable in Applied Mathematics, Computational Statistics, Computer Science, Physics, Electrical Engineering or related fields. Strong background in computational statistics, applied mathematics and statistical mechanics. Demonstrated knowledge in ML techniques, Monte Carlo methods, Molecular Dynamics, DFT. Good programming skills in C/C++, Python as well as good software development practices (e.g. version control software usage and embedded tests). Experience in high performance computing. Research experience in Applied Statistics in interdisciplinary applications (e.g.: Health, Energy).

#### Renefit

The gross annual salary of the Fellowship will be 28.000 - 32.000€. There is a moving allowance for those researchers that come from a research institution outside the Basque Country from EUR 1.000 to EUR 2.000 gross.