

**Date of publication of the job offer: September 10<sup>th</sup> 2021**

**Job Offer: PhD position - Machine Learning at the Computational Science Laboratory, University Pompeu Fabra, Barcelona**

**Job Description:**

Universitat Pompeu Fabra <http://www.upf.edu> and Prof. Gianni De Fabritiis, ICREA research professor <https://es.linkedin.com/in/gdefabritiis>, are looking to recruit a PhD candidate to contribute to understanding the underlying mechanism of intelligence behaviour towards machine intelligence applications.

Lab website: <http://www.compscience.org/>

Relevant References: [https://scholar.google.es/citations?hl=en&user=-kX4kMAAAAJ&view\\_op=list\\_works&sortby=pubdate](https://scholar.google.es/citations?hl=en&user=-kX4kMAAAAJ&view_op=list_works&sortby=pubdate)

**Aim:**

This project aims to develop machine learning models in physics and chemistry for enhancing the accuracy and simplicity of molecular simulation methods via active learning and end-to-end approaches.

**Location:**

The laboratory is located in the Barcelona Biomedical Research Park which, with a privileged location on the shoreline of the Mediterranean sea, constitutes one of the most exciting interdisciplinary research centres in Southern Europe with more than 1000 scientists in the building alone.

**Project and Institution that finance the contract** - The work is supported with H2020 European Commission Funds, by grant H2020-CompBioMed2-Gianni de Fabritiis

**Official number reference:** PREUR00419 - H2020-CompBioMed2-Gianni de Fabritiis

**Skills and Experience**

- The candidate will preferably have a profile in computer science, physics or mathematics. However, we seek exceptional candidates with a passion for computing, the capability to think out of the box, and the ambition to work in very innovative projects more than specific profiles.
- Very good communication skills in English.
- Previous experience in reinforcement learning and related fields, Python proficiency and coding skills, knowledge of Tensorflow or pytorch, familiarity with Linux and the ability to work with version control systems (e.g. git) are required.

**Facilities:**

Access to state of the art computational resources and large amounts of simulation data, which will be crucial for the development and validation of novel computational protocols. The lab is equipped with a cluster with state-of-the-art GPUs and has exclusive access to GPUGRID.net, a distributed computing project with 5000 GPUs.

