

**Postdoctoral Position PD2021MD- Deep Learning applied to Molecular Simulations
at the Computational Science Laboratory,
University Pompeu Fabra, Barcelona**

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 postdoctoral scientist to lead a research line in building and using machine learning potentials for molecular simulations. The candidate will contribute together with other PhDs fellows to the following research line of the Computational Science Laboratory (<http://www.compscience.org/>) :

Research line: Molecular simulations and machine learning. We use computation such as physics-based simulations and modern machine learning to provide novel, innovative methodological approaches in biomedicine. Specifically, we develop new methods that can be applied to drug design, protein dynamics, protein-protein interactions, etc. For this, we created GPUGRID.net in 2008, currently the second largest distributed computing project harnessing several thousands GPUs. In 2017 we created PlayMolecule, a publicly-available platform offering molecular simulations and machine-learning-powered assets for drug discovery used by a wide community of users (>100k jobs reached, >6000 unique users). The platform has been successfully tested in blind challenges (D3R challenge 2018, Sampl 2019) and it is currently deployed internally in several top-10 pharmaceutical companies. Since 2019, we are core project leaders of OpenMM/ACEMD, one of the leading molecular dynamics packages, jointly with the University of Stanford and the Memorial Sloan Kettering Cancer Center (NY,USA) where we are responsible for the development of machine learning potentials between quantum and classical mechanics and end-to-end simulation approaches.

This year we have released TorchMD, a framework for molecular simulations that enables users to do research faster in force-field development as well as integrate neural network potentials seamlessly into the dynamics with the simplicity and power of PyTorch.

Relevant References:

https://scholar.google.es/citations?hl=en&user=-_kX4kMAAAAJ&view_op=list_works&sortby=pubdate

Location:

The laboratory is located in the Barcelona Biomedical Research Park (PRBB) 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. The PRBB is more than just a research institution, it is a unique creative space that connects science and diversity. By becoming a member of its research community, the candidate will have access to conferences, networking opportunities and training events.

Candidate Profile:

- The candidate will preferably have a profile in chemistry, physics, computer science 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.

- The capability to think out of the box, the ambition to work in very innovative projects and very good communication skills in English.
- Previous experience in molecular simulations/quantum chemistry. Previous experience in machine learning potentials is beneficial.
- Python proficiency and coding skills, knowledge of Pytorch, familiarity with Linux and the ability to work with version control systems (e.g. git) are required.
- An excellent publication record during the PhD is positively evaluated

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.

****Eligibility:****

Please send an email to gianni.defabritiis@upf.edu with subject "JOB PD2021DL" with a CV and a cover letter together with the names of up to three contacts for references. recommendations

Salary:

We offer a competitive salary, depending on experience.

Duration:

Initially 1-year contract with the possibility of extension to 3 years in total

Deadline: Until filled - expected starting date anytime by the end of 2021