

# PhD and Postdoctoral positions on deep learning biomolecular simulations

Prof. Gianni De Fabritiis, ICREA research professor (<https://es.linkedin.com/in/gdefabritiis>)  
at the Computational Science Laboratory, University Pompeu Fabra, Barcelona

We are looking to recruit multiple positions at PhD and Postdoctoral levels to work **on next generation molecular simulations and neural network potentials with the goal of substantially impacting physics-based simulations and molecular dynamics.**

These positions involve having a key role in the development of OpenMM (<http://openmm.org>) of which we are co-coordinators. The candidate will contribute together with other PhDs fellows and international collaborators from academia and industry to the research lines of the Computational Science Laboratory (<https://www.compscience.org/>).

Relevant publications. [TorchMD: A deep learning framework for molecular simulations. S Doerr, M Majewski, A Pérez, A Krämer, C Clementi, F Noe, T Giorgino, ... Journal of chemical theory and computation 17 \(4\), 2355-2363](#)  
(<https://github.com/torchmd>)

## [Lab's publications](#)

**What you will do.** Depending on your skillset, you are expected to contribute to the machine learning of neural network representations for molecular potentials, improve speed in collaboration with OpenMM and Nvidia, enhance capabilities in terms of representing longer range physical terms, charges, etc.

**What you need.** The candidate will have a profile in physics, chemistry, computer science, or similar. We seek exceptional candidates with a passion for computing. Very good communication skills in English. A solid previous experience in ANY of the following:

- molecular simulations and quantum chemistry
- machine learning and PyTorch
- CUDA, C++ and very good coding skills
- Depending on the position an excellent publication record is positively evaluated

**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.

**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](mailto:gianni.defabritiis@upf.edu) with subject "PDPHD2021MD" with a CV and a cover letter together with the names of up to three contacts for references. We will contact you only if you are selected for a presentation.

**Salary.** We offer a competitive salary, depending on experience.

**Duration.** For the postdoctoral position this is a potentially long term position (up to 5 years). For the PhD is a 3 to 4 years position

**Start date:** Anytime from now