## **Open** position

## PhD position in Bioinformatics, Molecular Dynamics and Modeling available (BiMoDyM), CMLA, ENS Paris-Saclay (Cachan), France

Three-year PhD position in molecular modelling of enzyme and its activation within the ANR Project ROC (2019-2022)

We give talented and highly motivated student the opportunity to undertake PhD research at the cutting edge of modern biology, physics, mathematics and computer sciences.

The aim of the PhD project is to develop computer models of enzyme (native and mutants) embedded in lipid membrane and to simulate its activation by the partner protein. Computational methods will include protein-protein docking (classic and haptic), molecular dynamics simulations and quantum mechanics. The student will generate large-scale simulation data, understand and master various statistical methods for data analysis. The PhD student will develop a novel method to handle the dynamic nature of proteins regions involved in binding.

The project will be realized in collaboration with mathematicians for the methodological development and with biologists for the experimental validation of the predicted results.

Key Requirements: Master degree (or equivalent) in Bioinformatics, Physics or Mathematics that qualifies the candidate for doctoral studies at the ENS Paris-Saclay (ED INTERFACES). A structural biology background, programming skills (at least, R/python language and use shell script under Unix) and a sound understanding of protein modelling and molecular simulations are required.

To apply, please send a motivation letter, a resume, and a summary of the Master thesis.

Closing date for applications: May 1, 2019.

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