INTERNSHIP PROGRAM FOR INTERNATIONAL STUDENTS

INTERNSHIP SUBJECT FORM

Name of the Host Laboratory	Laboratory for Optics and Biosciences (LOB)
Website of the Host Laboratory	https://portail.polytechnique.edu/lob/fr/alexey-aleksandrov
Research Group	Theoretical biodynamics/microbial adaptation
Internship Supervisor	Alexey Aleksandrov
Internship Subject	Atomistic simulations of flavin-binding blue light photoreceptors
Student's level	☐ Advanced Undergraduate Students (3rd or 4th year) ☐ Master's students (1st or 2nd year) ☒ PhD students
Proposed Duration	☒ 3 months ☐ 4 months ☐ 5 months ☐ 6 months
Prerequisites	The student should possess an excellent skill in molecular biology and computational/structural biology. Previous experience with the Linux environment and computer simulation techniques is desired.
Internship description (max. 15 lines)	Flavoproteins are ubiquitous and participate in a wide range of biological functions. Their function normally relies on flavin cofactors, which can adopt different redox and protonation states. Among flavoproteins, light-oxygen-voltage (LOV) domains are photosensory modules found in photoreceptor proteins from all three domains of life. The goal of this internship is to help elucidating the signaling mechanism of a LOV domain protein and engineering of new LOV domain variants for molecular biology applications. In particular, the student will use computer simulations to access the atomistic details of the function of a recently discovered LOV domain from Chloroflexus aggregans. Molecular dynamics simulations will be performed for the protein complexed with the flavin chromophore in reduced and oxidized forms corresponding to the inactive (dark) and active (illuminated) states. The student will further apply free energy simulation techniques to characterize energetics of conformational changes related to the light-sensing function of the LOV domain. Computer simulations will be performed using local powerful GPU-accelerated machines as well as the national supercomputer (CINES). The results of computer simulations will be corroborated by experimental data, including high-resolution X-ray diffraction (published and unpublished) and spectroscopic data.

The boxes marked with cross implies eligible