Internship M2 PPN

from 2026 April 1st to 2026 July 31th

Title of the project: Sub-THz electric-field–driven dynamics of Conalbumin Protein

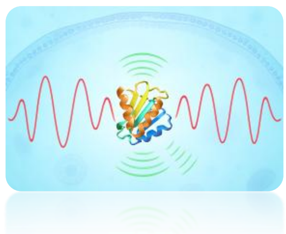
Supervisor(s): Adrien NICOLAÏ et Patrick SENET

Laboratory / Department / Team: ICB / Nano / Physics Applied to Proteins

Collaborations : Jérémie Margueritat (Institut Lumière Matière, Lyon)

Summary: Proteins are nanobioparticles essential for all biological processes in living organisms. According to the Anfinsen principle, the structure of a folded protein in a cell is encoded only by its amino-acid sequence and by the thermodynamical parameters of its environment. The structural properties define the protein function but how a protein functions also requires insight into its conformational dynamics. At physiological temperature, proteins exhibit a broad range of intrinsic motions spanning multiple temporal scales, governed by a complex multidimensional free-energy landscape. In particular, transitions between metastable substates, separated by free-energy barriers, typically occur on nanosecond to microsecond or longer timescales and are closely related to biological functions such as enzyme activity, molecular recognition, and protein–protein interactions.

Free-energy barrier crossing are related to protein collective modes. Many collective motions relevant to protein function can be described by a limited number of low-frequency vibrational modes, corresponding to acoustic modes in the sub-THz frequency range. As a result, there is a strong interest in identifying these acoustic vibrations and their role in biological activity. Information on protein vibrational modes in the (sub)-THz regime can be obtained from neutron, Raman, and Brillouin scatterings and by far-infrared spectroscopy. [1] Recently, Extraordinary Acoustic Raman spectroscopy has provided unprecedented access to the acoustical modes of proteins (< 100 GHz) [2]. In this technique, a single protein is trapped in a gold double nanohole and excited by two optical lasers of slightly different wavelengths, generating a low-frequency electric field (< 100 GHz). Despite its high spectral resolution, the physical mechanism governing excitation and the resulting structural response of the protein remain only partially understood and are thought to be linked to the modulation of electrostriction forces at the trapping site.



The objective of this Master internship is to investigate the dynamical response of the protein conalbumin using Molecular Dynamics simulations under oscillating electric fields in the 10–200 GHz frequency range. Simulations will be performed both in aqueous solution and in the presence of a gold surface, in order to assess the influence of the environment and of the substrate on the protein's low-frequency dynamics. The simulations will be compared with available experimental data from the literature [1] and will support the interpretation of future Brillouin scattering measurements [3] that will be performed by our collaborator.

[1] Nicolaï, A., Delarue, P., Senet, P. (2019). Raman and Infrared Spectra of Acoustical, Functional Modes of Proteins from All-Atom and Coarse-Grained Normal Mode Analysis. https://doi.org/10.1007/978-3-319-95843-9_15

[2] Wheaton, S., Gelfand, R. & Gordon, R. Probing the Raman-active acoustic vibrations of nanoparticles with extraordinary spectral resolution. *Nature Photon.* 9, 68–72 (2015). https://doi.org/10.1038/nphoton.2014.283

[3] Palombo, F. and Fioretto, D. Brillouin Light Scattering: Applications in Biomedical Sciences. Chem. Rev. 2019, 119, 7833−7847. https://doi.org/10.1021/acs.chemrev.9b00019

Type of project (theory / experiment): theory / computation

Required skills: Nanobiosciences, Molecular Dynamics, Proteins, Python for Data Analysis