

INTERNSHIP PROPOSAL

Laboratory name: IPCMS

CNRS identification code: UMR 7504, CNRS and University of Strasbourg

Internship director's surname: **Jérémie Léonard**

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Internship location: IPCMS, 23 rue du Loess (Bât. 69) 67037, Strasbourg.

Thesis possibility after internship: NO (funding requests have been asked)

Funding: YES ANR Project

Condensed Matter Physics: YES

Soft Matter and Biological Physics: YES

Quantum Physics: YES

Theoretical Physics: YES

Modeling ultrafast exciton transport in bio-inspired organic light-harvesting nanoparticles

Energy transport is a key process at play in natural photosynthesis [1]. Although pivotal to biology, this mechanism is still incompletely understood [2], but drives the interests of both fundamental and applied science. Indeed, natural photosynthesis involves that the energy absorbed from the sun is converted to an electronic excitation (EE, also called excitons) that is further transported over mesoscopic distances to a center where chemical reaction occurs. This EE transport takes places with near unit quantum efficiency, a fact which has inspired a lot of innovative applications including the design of synthetic materials for photovoltaic, photocatalysis, biosensing and chemical sensing [3].

This internship aims at increasing the understanding of artificial photosynthesis by performing a theoretical modeling of EE transport in organic, bio-inspired light harvesting (LH) systems. The model design and parametrization will be guided by time-resolved fluorescence spectroscopy experiments performed in IPCMS on synthetic polymer nanoparticles (NP; 40 nm in diameter) encapsulating a few thousand rhodamine fluorescent dyes [4]. The goal will be to compute quantitatively and to simulate (i) the fluorescence anisotropy decay, which reveals the time scale τ_{hop} for the ultrafast individual EE hopping events and (ii) the slower EE diffusion mechanism with a diffusion constant D [5] that is extracted from the fluorescence quenching.

For that purpose, we will derive a microscopic chemical rate equation (CME) [6] ruling the EE transport mechanism and solve it numerically using a Monte-Carlo (MC) simulation [7] from which the diffusion constant D can be extracted. A complementary analytical derivation through a Fokker-Plank equation [6,7] will be performed. More generally, we aim at unraveling the deep connection and interplay existing between the various time scales as encoded in the measured and computed τ_{hop} and D . This will be a first step towards a better understanding of EE transport, which is necessary to stimulate the emergence of innovative biomimetic photosynthetic materials. The candidate will join the IPCMS and work with **J. Léonard** performing the EE transport experiments and **R. Avriller** & **B. Bacq-Labreuil** working on the theory and simulation of EE transport. The candidate will benefit from a stimulating scientific environment in close connection between theory and experiments.

[1] Y.C. Cheng et al., [Annual review of physical chemistry](#), **60**(1), 241-262 (2009).

[2] A. Jha et al., [Chemical Society Reviews](#), **55**(2), 1089-1130 (2026).

[3] K. Kalyanasundaram et al., [Current opinion in Biotechnology](#), **21**(3), 298-310 (2010).

[4] K. Trofymchuk et al., [Nature Photonics](#) **11**, 657-663 (2017).

[5] A.M. Gharbi et al., [Nanoscale](#) **16**, 11550-11563 (2024).

[6] N.G. van Kampen, *Stochastic Processes in Physics and Chemistry* (1992).

[7] R. Avriller et al., *Phys. Rev. B* **108**, 205419 (2023).