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S E M I N A I R E

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" Phase behavior of thermo-responsive polypeptides "

Inspired by the aggregate formation in nature, the design of new materials with tailor-made properties received huge attention due to the broad range of their applications including the fabrication of responsive bio-interfaces, controlled drug-delivery, and release systems, etc. The use of intrinsically disordered protein-based polymers with high control over the protein sequence and length allows for finely tuning the corresponding phase behavior of the system. One example of such bio-polymeric materials is elastin-like polypeptides (ELPs) - artificially derived bio-polymers that mimic the hydrophobic repeat unit in the protein elastin. They typically exhibit a lower critical solution temperature (LCST) phase behavior in an aqueous environment characterized by an expanded-to-collapsed conformational change of a polypeptide chain. In this seminar, I will first present the hydrophobic collapse and assembly of a short ELP: Gly-Val-Gly-(Val-Pro-Gly-Val-Gly)$_3$ employing Molecular Dynamics simulations in conjunction with advanced sampling techniques with an atomistic resolution. In particular, I will discuss how the structural and dynamical properties of these ELPs vary as a function of the concentration in the vicinity of the transition, and which residues are essential for contact formation in multi-chain systems. In the second part of my talk, I will show how the conformational properties and free energy landscape of an ELP with the sequence (Val-Pro-Gly-Val-Gly)$_N$ changes as a function of the chain length in the temperature range relevant to ELP's application. Specifically, I will show that the number of intra-peptide hydrogen bonds, their spacing along the chain, and their lifetime depend on the peptide chain length. Such an analysis explains why short chains mostly visit extended conformations, i.e., coils, while the longer sequences prefer more compact ones, i.e., globules.

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14h30

Salle des conférences