Short Peptide Induced Gelation of Electrostatically Charged Supramolecular Assemblies

Our research focuses on the **symbiotic combination of experimental and computational methods** to design, understand, and optimize supramolecular peptide assemblies (SPAs) for certain applications (Figure 1).[1-2] We have successfully applied this combined approach in the past for the **optimization of artificial extracellular matrices for tissue regeneration** with great results in controlling the differentiation of human stem cells and in the regeneration of the spinal cord in mice.[3-4]

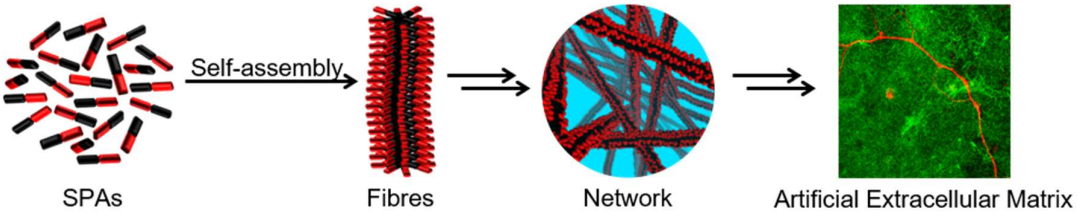

Figure 1. Scheme of the self-assembly of SPAs into Fibres, that then form a Network that gives rise to an Artificial Extracellular Matrix (with a neuron in red).

Objective

Based on newfound knowledge,[5-6] **we will develop short peptide co-assemblers (SPCs) with high affinity for the target SPAs, thereby enabling us to finetune surface and structure features to control interfilamentous interactions.** As these interactions determine mechanical properties and interactions with membranes, their control holds paramount importance **for their application as scaffolds for tissue regeneration and others such as catalysis.**

Training Program

The project´s computational/experimental balance will be **adapted to the candidate's interests**. The potential candidate does **not require previous knowledge in the field but a willingness to learn and work on a multidisciplinary project** at the intersection of computational chemistry, structural biochemistry, physics, and biology. The candidate will develop a deep understanding of the fundamentals of intermolecular interactions and supramolecular self-assembly, focusing on the **understanding and design of functional soft materials**. The candidate will have the opportunity to learn computational and experimental methods, including spectroscopic, microscopy, and other material characterization techniques. Additionally, we will **encourage the creativity** of the candidate to take the lead in the project and propose new directions.

Dr. Ivan Sasselli is **fully committed to the training and close supervision** of students with the purpose of adapting to them and giving guidance throughout their PhD. He has developed a strategy to follow the work and evolution of the students. The plan is not only intended for the PI to keep track of the student work but also to help the students to maintain a perspective of their progress and **acquire the skills needed to independently guide their own research**.

The student will attend international workshops and conferences to complement their skills and disseminate results. Additionally, as part of the UPV-EHU and CSIC, the student will have access to a wide range or training activities including MSc and PhD classes, PhD seminars, different Transversal Skills Programs (UPV-EHU, CFM, and DIPC), and CSIC courses.

References

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6. Sather, N. A., et al., *Small* **2021,** *17*, 2005743.

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