

Tuesday, 21st May, 12.00 pm, Seminar Room Host: Dr. Aitziber L. Cortajarena & Dr. Ivan Coluzza

Understanding Supramolecular Peptide Nanostructures

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Supramolecular peptide nanostructures are promising materials for nanomedicine and biotechnology applications. Although their properties can be tuned by changing the noncovalent interactions, the understanding of these materials at the intermolecular level is limited. Experimental methodologies are often incorrectly extrapolated from proteins and their interpretation is not straightforward, due to the lack of crystal structures to benchmark them. Computational methods have shown some potential in understanding and predicting self-assembly of peptides into nanostructures. However, the lack of experimental initial structures (e.g. crystals) and well-established methods make the validation of these results a major challenge. In my studies I show how a proper symbiosis between experimental and computational methods can be used to fill the gaps in each approach and achieve an otherwise inaccessible level of understanding of these systems. This synergistic approach has given us a unique insight into intermolecular order, superstructure formation, mechanical properties of the material, and the molecular mobility within supramolecular assemblies. With this information we can predict differences in viscosity, determine mechanisms of cell maturation on these substrates and, ultimately, design new functional materials for nanomedicine.