MATERIALS SCIENCE AND TECHNOLOGY

DISAT - Molecular Modelling of supramolecular systems response to concentration fluctuations

Funded By	Dipartimento DISAT
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Context of the research activity	This research aims to investigate the collective response of synthetic and natural supramolecular systems to concentration variations. The activities include the development and application of properly suited simulation strategies and elaborated data analysis techniques to characterize emerging collective phenomena in supramolecular materials when subject to concentration fluctuations.
	Vital functions of living materials occur in chemically non-uniform environments shaped by spatio-temporal concentration gradients. These gradients play a key role in influencing the structure and dynamics of biomaterials. For instance, the controlled self-assembly of natural supramolecular polymers—such as microtubules and actin filaments—or the phase separation of protein droplets in embryonic cells are striking examples of how chemical gradients orchestrate biological organization. Inspired by nature, materials scientists are designing synthetic supramolecular materials that offer a promising platform to mimic the dynamic, responsive, and functional behavior of living systems. Built from molecules that reversibly self-assemble into fibres, nanoparticle clusters, micelles, or droplets, these materials possess unique features like stimuli-responsiveness, self-healing, and structural tunability—essential for applications in organic electronics, medicine, molecular transport, catalysis, and more. Like their natural counterparts, the self-organization and adaptive behavior of synthetic supramolecular systems are influenced by concentration gradients. Yet, despite the fascinating implications of coupling self-organizing materials with chemical gradient modulations, our ability to precisely control their response to such gradients remains limited. The SYSMAGRAD project, the funding action supporting this PhD scholarship, applies advanced molecular modelling techniques to tackle this challenge. In the SYSMAGRAD framework, this PhD project aims at systematically exploring the behavior of stimuli-responsive supramolecular systems as the concentration of chemical species fluctuates. The main focus of the activities is to perform molecular dynamics (MD) simulations of relevant supramolecular systems at multiple scales,

Objectives	extensively varying the concentrations of constitutive and environment species, modelling both homogeneous and non-homogeneous conditions. Building on the simulation outcomes, a key goal is to elaborate an effective strategy to capture the collective response (in terms of structure and dynamics) of such materials to global and local concentration fluctuations, in an effort to draw general guidelines for a variety of different systems. The candidate will learn the most effective strategies to simulate supramolecular systems, and the methodologies that can be exploited to impart concentration fluctuations. Towards the goal of developing an effective analysis framework to highlight the emerging, collective response of supramolecular materials, the candidate will also learn to employ advanced structural clustering techniques and statistical analysis instruments to process the simulation data. The research activity will include: 1 – The multi-scale (atomistic and coarse-grained) molecular simulation of different supramolecular systems, from cooperative fibres to fuel-driven aggregates, immersed both in homogeneous and nonhomogeneous environment. 2– The elaboration of key analysis approaches to capture emerging collective properties in the simulated systems, by employing advanced structural clustering and statistical techniques on the simulation data output. 3 – The direct collaboration with experimental groups to favour the integration of modelling results within the experimental picture. The project operates at the frontiers between physics, materials science and chemistry, giving the opportunity to develop a strong expertise in the physics and statistical mechanics of complex systems, in molecular simulation techniques and in supramolecular science. The goals are relevant to a variety of synthetic and natural systems, ranging through multiple disciplines and possible applications, with the potential of very high impact results.

Skills and competencies for the development of the activity	Solid background in physics and/or materials science and/or chemistry and/or alike Strong interest in statistical mechanics and related topics. Strong motivation for scientific research. Preferable experience in molecular modelling and molecular simulation techniques (e.g., Molecular Dynamics, Monte Carlo, etc.) Preferable experience in analysis of complex data structures, clustering methods and related topics. Preferable experience in algorithm development and programming (C/C++, Python, etc.).