MATERIALS SCIENCE AND TECHNOLOGY

DISAT - Molecular Modelling of Supramolecular Materials in Chemical Gradients

Funded By	Dipartimento DISAT
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Context of the research activity	This research aims at the extensive molecular simulation of selected synthetic and natural supramolecular systems upon concentration gradients (such as co-solvent, ions, competitors), to unveil the coupling between emerging properties and nonhomogeneous chemical environment. The activities include the development of properly suited molecular models and their usage in molecular dynamics simulations. "Progetto SYSMAGRAD - FIS-2023-00936 - Bando FIS2 - CUP E53C24003790001".
	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. Within the framework of SYSMAGRAD action, this PhD project aims at investigating selected supramolecular systems via molecular dynamics, focusing on their coupling to the surrounding chemical environment, in

Objectives	particular when chemical gradients are sustained by the external conditions. The candidate will work at the forefront of research on self-assembling supramolecular materials, selecting systems that exhibit rich collective and dynamic behaviors. The project will explore how these materials interact with spatial and temporal concentration gradients of chemically active species, such as ions, fuels, or inhibitors. The main objective will be the comprehensive characterization of the dynamic, adaptive response of the supramolecular network when exposed to non-homogeneous chemical environments. The research activity will include: 1– An extensive survey of experimental state-of-the-art on responsive supramolecular systems, aimed at identifying common and fascinating collective phenomena associated with the presence of chemical gradients. 2 – The development of multiscale model representations of the relevant molecular species, to simulate in a reliable way both structure and dynamics of supramolecular assemblies 3 – Extensive molecular dynamics simulations based on these models, with the objective to extract trends, patterns and mechanistic principles governing the response of the supramolecular systems' structure and dynamics to imposed concentration gradients. The project operates at the frontiers between materials science, chemistry and physics, giving the opportunity to develop a strong expertise in supramolecular science and in the molecular simulation techniques that can be employed to obtain a detailed description of complex supramolecular systems. 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 chemistry and/or physics and/or materials science and/or alike. • Preferable experience in computational chemistry tools (DFT, tight-binding,…), toward the development of suitable molecular dynamics models (atomistic and/or coarse-grained). • Preferable experience in molecular dynamics simulation (e.g., GROMACS, LAMMPS, etc.) and relative data analysis. • Strong motivation for scientific research. • Preferable experience in Linux environment and High-Power Computing usage. • Good written and spoken English. • Ability to work both independently and as part of a team.