MATERIALS SCIENCE AND TECHNOLOGY

DISAT - Molecular Model and simulation of chemical-gradient-responsive Supramolecular Materials

Funded By	Dipartimento DISAT
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Context of the research activity	This research aims at developing molecular models of synthetic and natural supramolecular systems that display specific coupling concentration gradients of chemical species (such as co-solvent, ions, competitors) surrounding them. The activities include both the development of atomistic and coarse-grained models to capture multiscale aspects of the systems coupling with chemical gradients.
	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 framework of SYSMAGRAD action, this PhD project aims at tackling the study of various supramolecular systems via molecular dynamics (MD) simulations of the self-assembly and supramolecular equilibrium stages. The main focus of the activity is the definition of reliable molecular models for

Objectives	supramolecular polymer systems for the MD simulations with both atomistic and coarse-grained resolution. The candidate will investigate the state-of-the-art of self-assembling supramolecular materials that couple with concentration gradients of perturbing chemical species (ions, fuels, inhibitors). The main objective will be the parametrization of multiscale molecular models to be employed for MD simulations that could complement and extend experimental knowhow, particularly focused on the coupling of the supramolecular dynamics with concentration gradients. The research activity will include: 1– The survey of experimental state-of-the-art on responsive supramolecular systems, to identify those systems that display fascinating collective properties when subject to externally imposed chemical gradients. 2 – The development of atomistic model representations of the relevant molecular species to simulate structure and dynamics of supramolecular assemblies with high chemical detail. 3 – The development of Coarse-Grained models, building on the atomistic descriptions, retaining only the essential physico-chemical aspects to enable large space and timescale simulations. 4 – The extensive multiscale molecular dynamics simulations of different supramolecular systems, to observe the effects of concentration gradients on their structure and dynamics at different levels of detail. 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 materials science and/or chemistry and/or physics and/or alike. Preferable experience in molecular dynamics simulation (e.g., GROMACS, LAMMPS, etc.) and relative data analysis. Strong motivation for scientific research. Preferable experience in usage of molecular dynamics forcefields and development of molecular dynamics models (atomistic and/or coarse-grained). 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.