MATERIALS SCIENCE AND TECHNOLOGY

DISAT - Molecular simulations of self-assembling systems in chemical gradients

Funded By	Dipartimento DISAT
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Context of the research activity	This research aims to establish a computational framework for the molecular simulation of self-assembling molecular systems (such as supramolecular polymers and biomaterials) in the presence of spatio-temporal chemical gradients. The activities include both the development of new methodologies and the application of established algorithms, which will be validated on multiple systems of broad scientific and practical interest.
	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 such kind of phenomena remains limited. The SYSMAGRAD project, the funding action supporting this PhD scholarship, applies advanced molecular modelling techniques to tackle this challenge. In this framework, this PhD project aims at developing and establishing computational strategies to model the coupling between the dynamics of self-assembling molecular systems and chemical gradients. The main focus of the candidate activity consists in identifying reliable

Objectives	simulation protocols that, combining, e.g., Molecular Dynamics (MD) techniques, advanced sampling methods and Monte Carlo steps (such as insertion/deletion), allow the simulation of self-assembling molecular systems in the presence of stationary/dynamic chemical gradients. The candidate will learn how the existing methodologies to control the chemical potential in MD (such as e.g. CμMD, GCMC-MD , DCV-GCMD) can be adapted to the realm of self-assembling systems. This will include the extension of such methodologies and, possibly the elaboration of entirely new techniques. The research activity will include: 1 - the detailed understanding of the statistical mechanics describing such kind of molecular systems, both in equilibrium conditions and when the presence of gradients drives the system out-of-equilibrium. 2 – the implementation of ad-hoc algorithms, integrated in the MD engine, that can locally shape the system chemical potential to establish the desired chemical gradients. 3 – the validation of the engineered methodologies via simulation of both simple, paradigmatic self-assembling systems and more complex, frontier test-cases. 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 algorithm development and programming (C/C++, Python, etc.). 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