MATERIALS SCIENCE AND TECHNOLOGY

Ateneo - Advanced Computational Approaches for Self-Organizing Dynamic Materials

Funded By	Politecnico di TORINO [P.iva/CF:00518460019]
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Context of the research activity	This research will integrate molecular simulations, advanced descriptors, and machine learning to study and characterize the dynamics of self-organizing materials/systems. Focus is on analyzing large datasets extracted from molecular simulations to understand the properties of various systems. The project will involve multiscale simulations, data analysis, and models to predict emergent behaviors. This research aims at bridging the gap between molecular-scale phenomena and macroscopic behaviors.
Objectives	Complexity is ubiquitous in nature. Many natural materials and functional molecular systems are composed of fundamental units that recognize each other, interact, and self-assemble into complex structures having an innate dynamical character. In these systems/materials, the molecular building blocks continuously exchange between the assemblies that populate the system. The assemblies dynamically communicate with each other and with the external environment generating a dynamic molecular communication network and imparting to these systems fascinating properties, such as, e.g., the ability to change, reconfigure, or react dynamically in response to environmental variations or specific stimuli. In this perspective, understanding the key determinants that govern higher-scale structure and dynamics in these systems is essential but is also typically difficult. The aim of this PhD research is to investigate and model complex molecular systems and various types of dynamical self-assembling materials using a combination of molecular simulations and machine learning techniques. This research will focus on the development of advanced data-driven analyses and of unsupervised machine learning approaches to extract - from large datasets obtained from, e.g., molecular simulations - clear insights into the fundamental factors that control the properties emerging into various types of self-assembling materials and complex molecular systems. The PhD candidate will develop atomistic and coarse-grained models and use different types of molecular simulation approaches to study a variety of self-organizing molecular systems and materials. Machine learning approaches will be then used to understand the key factors that control the properties that emerge within them. To this end, the candidate will develop

	and use methods such as, e.g., advanced physical descriptors, dimensionality reduction, unsupervised clustering, pattern recognition, times-series analyses, causality relationships, etc. These approaches will help identifying the factors that influence the behaviors and the properties of these materials. This will pave the way toward the rational design of new types of molecular and supramolecular materials/systems with programmable dynamic behaviors, which is the long-term objective of this research. Systems of interest will include, e.g., supramolecular fibers, tubes, vesicles, micelles, as well as metal or polymeric systems that possess fascinating innate dynamical behaviors. The PhD candidate will combine atomistic and coarse-grained models with classical and advanced molecular simulations (e.g., molecular dynamics, metadynamics, etc.), as well as she/he will use machine learning approaches to convert the data extracted from the simulations into human-readable information useful for the rational design of new types of systems/materials. The computational research conducted by the selected PhD candidate will also benefit from the multiple interdisciplinary collaborations that our group has with pioneering scientists worldwide, which provides a rich environment for scientific development and innovation.

Skills and competencies for the development of the activity	Preferable skills are: • Experience in molecular modeling & simulation (molecular dynamics, etc) • Strong motivations to scientific research • Good background in chemistry, physics & materials science • Good programming skills (python, etc) • Experience in the Linux environment • Experience in machine learning • Experience in data-driven analyses • Experience in the use of advanced structural/dynamical descriptors • Good written & spoken English • Good attitude to work in team & independently