Séminaire

INSTITUT Charles SADRON
CNRS - UNISTRA - STRASBOURG

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Amphithéâtre Henri Benoît

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Towards AI driven design of metallo-supramolecular polymer networks

Towards AI driven design of metallo-supramolecular polymer networks Nature employs a wide array of transient interactions to operate adaptively on various time and length scales. Inspired by such elegant designs, combinations of different supramolecular assemblies have been extensively introduced in synthetic material platforms to obtain biomimetic functions. Among the most widely used transient bond, metal–ligand coordination plays a distinct role in designing robust and stimuli-responsive transient polymer networks. The functionality of the metal–ligand complex, combined with the technological benefits of the polymer backbone, provides novel materials with outstanding potential to be used in a wide range of applications. The knowledge of controlling the spatial configuration of supramolecular coordination complexes (SCCs) has been extremely advanced in recent years. Notable outcomes include, but are not limited to, the development of highly ordered static supramolecular arrays like metal-organic cages and frameworks as well as the advent of reversible molecular movements used in molecular machines. This wealth of knowledge has been rarely employed in the field of polymer science, which would otherwise offer a new approach to building highly ordered model-type networks or even inducing novel structural rearrangements in response to external stimuli. Addressing this gap, I have utilized a flexible platform that allows varying the coordination geometry and functionality of junctions and study the consequences on the macroscopic scale. I have demonstrated that the formation of heteroleptic complexes using self-sorting mechanisms developed for SCCs can provide polymer networks with structure and dynamics incomparable to the parent homoleptic networks. Same mechanism has been employed in the development of the first artificial muscle, where homo- and heteroleptic complexations induced molecular expansion and contraction. More recently, heteroleptic SCCs have been used in polymer science either to induce dynamic self-assembly into various nanoscopic morphologies and structures or to form stimuli-responsive network topologies. These advances at the interface of SCCs and polymer science could open new avenues for the development of macromolecular machines. An important question here is the effect of polymeric connectivity on the dynamics of such structure formation and stimuli-responsiveness, which I am currently investigating using fluorescence resonance energy transfer (FRET). The design space of SCCs is extensively wide and almost impossible to explore without computational effort and machine learning (ML). This forms the basis of my next 5-years research plan focused on the computational design of SCCs and the application of ML and modeling to experimentally validate the customized design of transient polymer networks for specific applications.

Les personnes souhaitant rencontrer M. Ahmadi sont priées de prendre contact avec Daniel Grande.