Institute of Science and Technology Austria

Innate Dynamics, Molecular Communication Networks & Emergent Bioinspired Properties in Complex Supramolecular Systems

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Supramolecular polymers, composed of monomers that self-assemble via non-covalent interaction into 1D, 2D, or 3D structures (or materials) are attracting increasing interest in many fields.[1] In such self-assembled systems, the constitutive building-blocks obey to a well-defined supramolecular equilibrium.[2] This imparts an intrinsically dynamic character to the assemblies that populate the system, which exist as exquisitely statistical/dynamical entities in continuous communication with each other and with the external environment, generating de facto a complex molecular system.

While typical experimental approaches allow to obtain average ensemble information on the dynamics of the entire system,[3] advanced simulation approaches may provide submolecular resolution insights into the origin of the dynamics of the (individual) assemblies.[4] However, the key molecular factors that control the communication networks and emergent properties in these complex molecular systems remain most often unclear. Learning how to master such complex molecular systems requires to enter into their innate dynamics at a submolecular resolution, and to obtain information on the molecular processes that control them.

In this talk, I will provide an overview of the computational approaches that we are recently adopting to reconstruct the intrinsic dynamics of self-assembling molecular systems. This journey brought us into the study of their complexity,[5] of their fluctuations,[6] and into the design and development of data-driven approaches to compare and classify them.[7] We are coming out with a new perspective, which contains general concepts that can be transferred to a variety of complex molecular systems and holds great potential for many applications.

Thursday, May 12, 2022 at 11am

Heinzel Seminar Room / Building West

This invitation is valid as a ticket for the IST Shuttle from and to Heiligenstadt Station. Please find a schedule of the IST Shuttle on our webpage: ttps://ist.ac.at/en/campus/how-to-get-here/ The IST Shuttle bus is marked IST Shuttle (#142) and has the Institute Logo printed on the side.