THEORETICAL STUDIES ON THE KINETICS AND DYNAMICS OF LIVING POLYMERS

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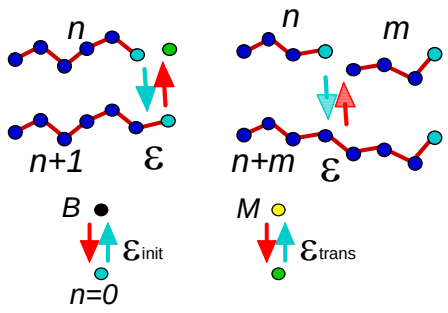
Classical polymers are built with chemical bonds that are practically permanent. By contrast, living polymers (LPs) involve *reversible* bonds permitting variations of the polymerization degree. The family of LPs (equilibrium polymers, dynamic and supra-molecular polymers) is very broad: it includes chains with covalent bonds (formed e.g. by step-growth polymerization or by such addition polymerization processes that avoid termination of the growing chains), living surfactant wormlike micelles, columnar structures of discotics (dyes, chromonics), supramolecular structures of proteins and peptides (tapes, fibrils, fibres, filaments like F-actin, microtubules), etc. LP structures are widespread in biological systems and are of rising importance for various materials science applications. LPs show versatile properties since the reversible bonds can be responsive to the environment and to external triggers.



In the general case the living chain growth kinetics is controlled by many factors like the unimer pre-association transformations, position-dependent scission and recombination rates, the presence of growth initiators and inhibitors. The main goal of the project is to assess the role of these factors for the dynamics of molecular-weight distribution and concentration fluctuations in LP systems. Such studies yielding the dynamical scattering functions (structure factors) of LPs are important for understanding and predicting their mechanical, rheological and other properties.

The work on the project will consist in theoretical (analytical, numerical, and computer simulation) studies of the LP dynamics following the general approaches of refs [1-3]. In particular, it will be necessary to analyse systems of entangled kinetic equations using both analytical and numerical methods. Considerations of the effects of chain stiffness, of multi-strand filament structures and of the seeding effects for fibrillization kinetics are anticipated as well.

The candidate must be familiar with the theory of polymer dynamics and have a solid background in basic mathematical (numerical) methods to solve differential equations.

[1] I. A. Nyrkova, A. N. Semenov. *The European Physical Journal E*, **2007**, v. 24, p.167.

[2] I. A. Nyrkova, A. N. Semenov, *Phys. Rev. E* , **2007**, v.76, # 011802.

[3] A. N. Semenov, *Physica A*, **1990**, v.166, p.263.