

Skoltech and Interdisciplinary Scientific Center Poncelet announce a minicourse

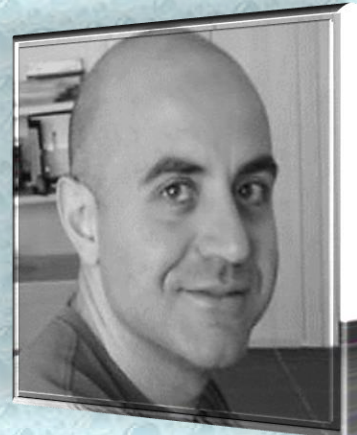
Computer Simulation of Polymers: Entanglements and Topological Constraints

Ralf EVERAERS
(ENS, Lyon, France)



Computer simulations of
entangled polymers

Angelo ROSA
(SISSA, Trieste, Italy)



From eukaryotic chromosomes to
physics of crumpled ring polymers

May 27-28, 2019

Independent University of Moscow, room 401, 10⁰⁰ - 16³⁰
Bolshoy Vlasievsky pereulok, 11

May 27: 10:00 – 11:30: Ralf Everaers
12:00 – 13:30: Ralf Everaers
15:00 – 16:30: Angelo Rosa

May 28: 10:00 – 11:30: Angelo Rosa
12:00 – 13:30: Ralf Everaers
15:00 – 16:30: Angelo Rosa

Ralf Everaers, **Computer simulations of entangled polymers** (three lectures)

Diffusing polymers can slide past each other, but their Brownian motion is subject to transient topological constraints, since the chain backbones cannot cross. The microscopic «entanglements» dominate the characteristic viscoelastic behavior, which polymers display macroscopically. In my lecture, I will first review the Rouse and the Edwards/de Gennes tube models of polymer dynamics. In the second part, I will introduce the Kremer-Grest bead-spring model and computational techniques used for simulating these generic model systems. The central part of the lecture focuses on the question, how computer simulations can be used to explore the physics underlying the tube model. In the final part, I discuss how to design *material-specific* Kremer-Grest models for commodity polymer melts.

Angelo Rosa, **From eukaryotic chromosomes to physics of crumpled ring polymers** (three lectures)

In these lectures, I will first introduce the audience to the relevant phenomenology of chromosome organization inside the nuclei of eukaryotic cells. Then, by employing simple and generic physical arguments, I will discuss how chromosome folding can be understood based on the analogy to unknotted and unlinked ring polymers which adopt "crumpled" conformations in dense solutions. The explanation of this analogy will offer the opportunity to discuss in detail the rich phenomenology of ring polymers: in particular, I will report about recent theoretical and computational work addressing the debated connection between ring polymers and melts of branched polymers.