**CA17139 “EUTOPIA” – Report of activities of WG2: Polymeric and fibrous topological materials (leader: Prof. Achille Giacometti (Venice University, Italy); co-leader: Dr. Angelo Rosa (Sissa, Trieste, Italy)).**

WG2 brings together theoretical and experimental competences devoted to the development of efficient large-scale computer simulation tools and the fabrication of nanodevices for characterizing the properties of soft matter systems where entanglement and topological properties play a fundamental role.

The activities of WG2 are intrinsically inter- and cross-disciplinary: they extend their influence on the activities of other WG’s, most notably those of WG3 (entangled and self-entangled proteins) and WG4 (DNA, chromosomes, and other entangled genetic material).

**Summary of recent activities.** The WG2 session organized during the recent (Feb. 2019) EUTOPIA First Meeting held in Trento (Italy) was inspired by these principles, and by the COST commitment to guarantee an as-much-as-possible adequate representation in terms of gender balance and target Countries.

The speakers of the section were selected by the group leaders along these lines and were instructed to provide an overview of one particular aspect of topics of interest for the working group.

The session lasted about 3 hours and was divided unto two sub-sections on “Topological Effects in Generic Polymer Systems, Coarse-Grained Polymer Models, Active Polymers” and on “Polymeric Gels, Characterization of Biopolymer Topological Properties (Linking Number, Torsion, Writhe, …)”.

Each part (90 minutes) was so planned: the first 60 minutes were dedicated to 2 ‘long’ talks of 15 minutes each, followed by 4-5 ‘short’ talks of 5 minutes each. As anticipated, each talk was meant to present the ‘state of the art’ of the subject, rather than the speaker’s personal research interests. Then, the remaining 30 minutes were dedicated to a ‘round table’ involving all speakers and focusing on open questions and perspectives. This formula proved very successful, with the speakers receiving many interesting remarks and insightful observations. Some of those are reflected in the list of projects, collaborations and STSM’s established during the event, which will be briefly summarized in the following.

The list of speakers and topics discussed during the WG2 session were the following:

1) Andrey Milchev (Germany), Topological aspects in polymer systems under geometric confinement.

2) Enzo Orlandini (Italy), Random knotting and linking.

3) Jan Smrek (Austria), Non-equilibrium thermally-induced phase separation in polymers.

4) Emanuele Locatelli (Austria), Self-propelled polymers: overview and perspectives.

5) Luca Tubiana (Austria), Polycatenanes and the kinetoplast DNA.

6) Davide Michieletto (UK), Ring polymers.

7) Mark Miller (UK), Coarse-grained methods for molecular and colloidal systems.  
8) Ivan Coluzza (Spain), A multi-scale approach to the study of protein design, folding and aggregation.

9) Kalina Peneva (Germany), Experimental polymer design for drug delivery.

10) Felix Schacher (Germany), Polymer chemistry: control freaks and how does this relate to topology?

11) Marina Scarpa (Italy), Cellulose nanocrystals: the building blocks for entangled wire-shaped materials.

12) Pavlos Stefanou (Greece), Entanglement effects in polymer melts and solutions: where we stand and what can be done.

13) Angel Moreno (Spain), Simulations of reversible and irreversible complex polymer networks: from to micro/nanogels to single-chain nanoparticles.

**Summary of open questions and future activities (including STSM’s).**

1) STSM (by April 2019): Jan Smrek (Vienna, Austria) is planning to visit Davide Michieletto in Edinburgh (UK), working on the structure and dynamics of ring polymers in melt which will be analyzed in terms of inter-ring threadings. This is a timely problem in polymer physics: both researchers are at early-stage career, they have developed their own complementary analysis tools which they wish to bring together to provide a unifying theoretical framework. The topic has relevance to the Physics of chromosomes inside the nuclei of the cells and hence is connected to the topics of WG4.

2) Aurica P. Chiriac (Iasi, Romania) is working on designing novel polymer networks containing: (1) copolymers with pendant spiroacetal moieties; (2) natural polymers; (3) low molecular mass gelators. These are promising materials due to their unique properties. In particular, the spiroacetal moiety is known to undergo a conformational change allowing for specific interactions related to the environment.

3) Pavlos Stefanou (Nicosia, Ciprus) is planning to extend current theories of tube models for entangled polymer systems by resorting to non-equilibrium thermodynamics able to account for the shear-induced migration towards surfaces. A particular emphasis will be paid to bidisperse systems.

4) Peter Virnau (Mainz, Germany) is planning to investigate self-entanglements in polymer melts, which have been largely ignored in polymer theory, but may nevertheless influence material properties. Recently, it was demonstrated that standard polymer models overpredict the occurrence of knots in melts, thus raising questions about their validity. In the next months, his group plans to build upon this work so to improve coarse-grained models of polymers based on soft potentials. He will also consider the effect of confinement on self-entanglements in polymer films.

5) Emanuele Locatelli (Vienna, Austria) is planning two STSM’s. He will visit first Valentino Bianco in Madrid (Spain). The intention is to study the self-entanglement (knotting) properties of active, i.e. out-of-equilibrium, polymer chains with the goal of quantifying how much these properties deviate from the common case at equilibrium. The second STSM is planned in Sissa (Trieste) in the group of Angelo Rosa, with the purpose of studying the physics of active polymer rings in the melt. Here, the idea is to monitor the time evolution of these systems moving from different initial states with the purpose of highlight and then quantifying non-equilibrium effects.

6) Marina Scarpa (Trento, Italy) is planning to focus on cellulose nanocrystals (CNCs) and cellulose nanofibrils (CNFs). These are sustainable nanomaterials undergoing self-assembly processes and forming transparent homogeneous suspensions and gels in aqueous media, and films in dried state. Moreover, they display different micro and macroscopic properties, depending on the experimental conditions such as concentration, crystallinity, charge and presence of solvent and salts. Some investigations report that they are able to self‐organize, owing to a yet-not-well-understood balance between orientation‐dependent attractive (van der Waals forces) and repulsive (steric or electrostatic, short and long range) interactions. To clarify these issues, Scarpa’s group proposes to investigate: (1) the physical conditions (particle-particle interactions and the relation to particle shape) which favor the CNC entanglement in solution and of the macroscopic structure and properties of the materials resulting from the CNC arrangements; (2) the dynamic conditioning of the CNC assembly process under shear flow for bulk and confined systems. Within the COST initiative, Scarpa’s group is encouraging the development of theoretical/computational approaches to understand the microscopic physical structure at the basis of these systems.

6) Three groups (Mark Miller in Durham, Ivan Coluzza in San Sebastian, and Achille Giacometti in Venice) are planning reciprocal visits through STSMs with the aim of applying free energy landscape theory to two recently developed coarse grained models. The expected outcome of this collaboration would be a bridge between the two models, as well as a better understanding of their transitional states.

7) One or more STMSs are planned between the group of Achille Giacometti in Venice and the group of Maria Barbi in Paris, to work on the liquid crystal properties of nucleosomes.