Symposium Topological constraints in biological and synthetic soft matter (SYSM)

jointly organised by
the Chemical and Polymer Physics Division (CPP),
the Biological Physics Division (BP), and
the Dynamics and Statistical Physics Division (DY)

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This focus session illustrates the importance of topology-related phenomena and processes in various areas of soft matter physics. The examples cover topological constraints in synthetic and biological polymer melts and gels, the role of knots in proteins, and topological defects in liquid-crystalline materials.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Sessions

SYSM 1.1–1.5	Mon	10:00–12:45	Audimax 1	**Topological constraints in biological and synthetic soft matter**

SYSM 1: Topological constraints in biological and synthetic soft matter

Time: Monday 10:00–12:45 Location: Audimax 1

Invited Talk SYSM 1.1 Mon 10:00 Audimax 1
Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation — •Alexandra Zidovska — Center for Soft Matter Research, New York University, New York, NY, USA

Cell differentiation, the process by which stem cells become specialized cells, is associated with chromatin reorganization inside the cell nucleus. Here, we measure the chromatin distribution and dynamics in embryonic stem cells *in vivo* before and after differentiation. We find that undifferentiated chromatin is less compact, more homogeneous and more dynamic than differentiated chromatin. Further, we present a noninvasive rheological analysis using intrinsic chromatin dynamics, which reveals that undifferentiated chromatin behaves like a Maxwell fluid, while differentiated chromatin shows a coexistence of fluid-like (sol) and solid-like (gel) phases. Our data suggest that chromatin undergoes a local sol-gel transition upon cell differentiation, corresponding to the formation of the more dense and transcriptionally inactive heterochromatin [Eshghi I, Eaton JA and Zidovska A, *Phys. Rev. Lett.*, 126(22): 228101 (2021)].

Invited Talk SYSM 1.2 Mon 10:30 Audimax 1
Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids — •Jan Smrek[1], Jonathan Garamella[2], Rae Robertson-Anderson[2], and Davide Michieletto[3,4] — [1]Faculty of Physics, University of Vienna, Austria — [2]Department of Physics and Biophysics, University of San Diego, USA — [3]School of Physics and Astronomy, University of Edinburgh, UK — [4]MRC Human Genetics Unit, Institute of Genetics and Molecular Medicine, University of Edinburgh, UK

Ring polymers in dense solutions are among the most intriguing problems in polymer physics. Thanks to its natural occurrence in circular form, DNA has been extensively employed as a proxy to study the fundamental physics of ring polymers in different topological states. Yet, torsionally constrained – such as supercoiled – topologies have been largely neglected so far. Here we address this gap by coupling large-scale Molecular Dynamics simulations with Differential Dynamic Microscopy of entangled supercoiled DNA plasmids. We discover that, unexpectedly, larger supercoiling increases the size of entangled plasmids and concomitantly induces an enhancement in DNA mobility. These findings are reconciled as due to supercoiling-driven asymmetric and double-folded plasmid conformations which reduce inter-plasmids entanglements and threadings. Our results suggest a way to topologically tune DNA mobility via supercoiling. In addition, I will highlight the importance of threading topological constraints in other complex polymeric fluids in- and out of equilibrium.

15 min. break

Invited Talk SYSM 1.3 Mon 11:15 Audimax 1
Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges — •Dimitris Vlassopoulos — FORTH and University of Crete, 100 N. Plastira St., Heraklion 70013, Greece

One of the biggest successes of soft matter physics has been the understanding of the rheological consequences of polymeric entanglements. It has set the stage for further advances which continue to date. Examples range from the viscoelastic spectrum of wormlike micelles to shear thinning of entangled polymers. Yet, a number of outstanding challenges remain, and here we present recent work addressing two of them: (i) Entangled linear polymers under strong shear exhibit a rich transient response whose interpretation remains controversial. We focus on the weak undershoot following the (well understood) overshoot of shear stress growth coefficient, which is often hard to detect experimentally. Modeling provides a rationalization by invoking the idea of tumbling which itself stems from simulation results. We designed a set of experiments with homopolymer blends to further elucidate its origin and identify the experimental and molecular parameters governing its appearance. (ii) Supramolecular assemblies based on hydrogen bonding motifs in apolar solvents exhibit rheological signatures which sensitively depend on traces (0.01%wt) of dissolved water. Hence, the relative humidity affects the viscoelastic response of the formed physical networks. We present results from linear and nonlinear rheometry which allow to quantify this overlooked effect and provide the ability to tune the rheology of supramolecular networks at molecular level.

Invited Talk SYSM 1.4 Mon 11:45 Audimax 1
Supercoiling in a Protein Increases its Stability — •Joanna Sulkowska and Szymon Niewieczerzał — Centre of New Technologies, University of Warsaw, Banacha 2c, 02-097 Warsaw, Poland

Currently it is known that at least 6% of proteins possess nontrivial topology (i.e. are entangled) and form structures called knots, slipknots, lassos, links and theta curves. A lasso is a structure that contains a covalent loop (closed by a cysteine, amide, or other bridge), crossed by at least one free end of a protein.

The supercoiling motif is the most complex type of nontrivial topology found in proteins with lasso motif. Based on a protein from extremophilic species with such a motif, with a coarse-grained protein model I will show that this protein can knot itself; however, the supercoiling changes a smooth landscape observed in reduced conditions into a two-state folding process in the oxidative conditions, with a deep intermediate state. The protein takes advantage of the hairpin-like motif to overcome the topological barrier and thus to supercoil. I will also show that the depth of the supercoiling motif, i.e. the length of the threaded terminus, has a crucial impact on the folding rates of the studied protein. Finally, I will show that fluctuations of the minimal surface area (i.e. the area of a surface spanned on a covalent loop) can be used to measure local stability, and that supercoiling motif introduces stability into the protein. These results suggest that the supercoiling motif enables the studied protein to live in physically extreme conditions, which are detrimental to most life on Earth.

Invited Talk SYSM 1.5 Mon 12:15 Audimax 1
Topology for soft matter photonics — •Igor Musevic — J. Stefan Institute, Ljubljana, Slovenia

Topological defects in liquid crystals can be created by either rapid pressure or temperature quench across the isotropic-liquid crystal phase transition and are stabilized either by colloidal inclusions or confinement. Defects appear as point charges or small defect loops that carry integer topological charge. Because the total topological charge must be conserved, point charges and loops in nematic liquid crystals always appear in pairs with opposite topological charges or in chargeless loops. Topological defects in liquid crystals can be used to assemble and even knot and link colloidal structures and superstructures of particles dispersed in a liquid crystal with the colloidal binding energy of the order of several 1000 kT. It has been also shown that micro-droplets of liquid crystals are in fact optical micro-cavities that can be put into laser operation solely by light. Because of the fluid nature of liquid crystals, droplets can be self-transformed into liquid fibers that are excellent optical wave-guides. This makes it possible to realize complex photonic devices, where topological defects act as a binding matter and the liquid crystal has the role of photonic soft matter.