CPP 60: Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers I (joint session BP/CPP, organized by CPP)

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The topological, or knotted, state of long chains influences their physical properties. Mechanical features of polymers and fibers, such as energy dissipation and tensile rupture, are known to be substantially affected by the presence and type of a knot. Entanglements have emerged as relevant players also in the realm of biophysics, as knots have been found in circular DNA as well as in proteins. In the last few decades a great effort has been put in the characterization of the properties of chains featuring a self-entangled topology. A large contribution has been provided in particular by computer simulations of knotted polymers, with a spectrum of different models and systems spanning from ideal chains to atomistic proteins and coarse-grained chromosomes. Furthermore, the advancement of experimental techniques has enabled researchers to construct, handle, and study physical knots, making possible a productive interplay between theory, computer modeling, and experimental validation. The scope of this focus session is to bring together scientists active in the multifaceted field of polymer topology, and foster the exchange of ideas among different areas. In particular, it is our aim to promote the interaction between two communities, polymer science and biophysics, that have insofar manifested a great collaborative potential.

Time: Thursday 15:00–18:00 Location: ZEU 260

Invited Talk CPP 60.1 Thu 15:00 ZEU 260

Polymers in the cell nucleus — •Maria Barbi, Antony Lesage, and Jean-Marc Victor — Laboratoire de physique Theorique de la Matiere Condensee - UPMC - Paris VI - France

Understanding the genome functional architecture and its dynamics is one of the big challenges of systems biology. The three-dimensional arrangement, in the cell nucleus, of the protein-DNA assembly that constitutes chromosomes is expected to be crucial for the regulation of gene expression, hence cell differentiation and cell type setting. The rapid progress of experimental techniques Begins to make it possible to explore these complex structures. I will show how, when used in connection with experimental results, polymer physics represents a powerful tool in deciphering the chromosome arrangement and dynamics.

CPP 60.2 Thu 15:30 ZEU 260

Minimal surfaces on unconcatenated polymer rings in melt — •Jan Smrek[1] and Alexander Grosberg[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Center for Soft Matter Research and Department of Physics, New York University, New York, NY 10003, USA

In order to quantify the effect of mutual threading on conformations and dynamics of unconcatenated and unknotted rings in the melt we computationally examine their minimal surfaces. We found a linear scaling of the surface area with the ring length. Minimal surfaces allow for an unambiguous algorithmic definition of mutual threading between rings. Based on it, we found that although ring threading is very frequent, vast majority of cases correspond to very short loops. These findings explain why approximate theories which neglect threading in the description of static and dynamic properties of ring melts are so unexpectedly successful despite having no small parameter justification. We also examine threading dynamics, and identify the threading order parameter that reflects the slowdown of the ring diffusion.

CPP 60.3 Thu 15:45 ZEU 260

Density effects in entangled solutions of linear and ring polymers — •Negar Nahali and Angelo Rosa — SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste, Italy

We present here recent [1] findings from molecular dynamics computer simulations regarding the statics and dynamics of linear and circular (ring) polymer chains in entangled solutions of different densities.

While we confirm that linear chain conformations obey Gaussian statistics at all densities, rings tend to crumple becoming more and more compact as the density increases. Conversely, contact frequencies between chain monomers are shown to depend on solution density for both chain topologies.

The relaxation of chains at equilibrium is also shown to depend on topology, with ring polymers relaxing faster than their linear counterparts. Finally, we discuss the local viscoelastic properties of the solutions by showing that the diffusion of dispersed colloid-like particles is markedly faster in the rings case [1,2].

[1] N. Nahali, A. Rosa, Journal of Physics: Condensed Matter 28, 065101 (2016)

[2] N. Nahali, A. Rosa, in preparation.

CPP 60.4 Thu 16:00 ZEU 260

Slow diffusion of ring polymer melts originated from inter-ring threading — •Eunsang Lee[1,2] and YounJoon Jung[1] — [1]Department of Chemistry, Seoul National University, Seoul 08826, Korea — [2]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle 06120, Germany

Topological constraints of a ring, nonconcatation and unknotting, force the rings to be in a threading configuration, which is believed to be a main reason for abnormally slow diffusion observed in a melt phase. In this presentation, we provide results for the threading dynamics using molecular dynamics (MD) simulation based on a bead-spring model and Monte Carlo simulation on a kinetically constrained lattice gas model. Threading configuration between two molecules frequently observed in MD trajectories causes asymmetric dynamic state of two molecules and a set of such rules is implemented in the lattice model to describe the ring diffusion. Both models well describe long-time behavior of the ring diffusion strongly governed by a long-lasting molecular contact from threading configuration. An evidence for the glassy dynamics is also presented to support the ring melt belonging to a topological glass. From this work, we gain physical insights on the relation between molecular topology and its slows dynamics of ring polymer melts.

CPP 60.5 Thu 16:15 ZEU 260

Topological Interactions in Dilute Polymer Solutions – Disentanglement of Two Single Chains — •Diddo Diddens[1], Nam-Kyung Lee[2], Sergei Obukhov[3], Jörg Baschnagel[1], and Albert Johner[1] — [1]Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France — [2]Institute of Fundamental Physics, Department of Physics, Sejong University, Seoul 05006, Korea — [3]Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611-8440, United States

The non-crossing constraint of individual polymer chains is a well-known feature that explains several dynamical characteristics of dense polymer solutions or melts. However, the situation becomes less clear when dealing with an ensemble consisting of only a few long polymer chains that overlap, a scenario that is frequently encountered in *e.g.* biopolymer physics. To assess the impact of topological constraints in dilute polymer systems in a general manner, we devise a hypothetical experiment in which a long polymer chain is cleaved into two distinct halves that initially overlap, and study their subsequent disentanglement via Molecular Dynamics simulations [1]. We demonstrate that the non-crossing constraint significantly affects the separation dynam-

ics, and quantify the associated relaxation times in terms of the topological properties of the starting configuration from which the cleavage is initiated. Moreover, we rationalize our findings by analytical arguments.

[1] D. Diddens *et al.*, *ACS Macro Lett.*, **2016**, 5(6), 740-744

15 min break

Invited Talk CPP 60.6 Thu 16:45 ZEU 260

Knots as Stable Topological Order Parameter for Semiflexible Polymers — •Wolfhard Janke and Martin Marenz — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We investigate the influence of bending stiffness on the conformational phases of a semiflexible bead-stick homopolymer and present the pseudo-phase diagram for the complete range of semiflexibility, from flexible to stiff. By varying the internal bending stiffness, the model exhibits different pseudo phases like bent, hairpin or toroidal. In particular, we find thermodynamically stable phases characterized by knots of specific topologies. The transitions into these "knotted" phases from other ordered phases are quite unusual in that they display clear phase coexistence but almost no change in the mean total energy and hence no latent heat. It will be explained how we arrive at these intriguing results by computer simulations based on a combination of the replica-exchange Monte Carlo algorithm and the multicanonical method and discussed how one can understand these effects by basic statistical physics reasoning.

M. Marenz and W. Janke, *Knots as a Topological Order Parameter for Semiflexible Polymers*, Phys. Rev. Lett. **116**, 128301 (2016).

M. Marenz and W. Janke, *Stable Knots in the Phase Diagram of Semiflexible Polymers: A Topological Order Parameter?*, J. Phys.: Conf. Ser. **750**, 012006 (2016).

CPP 60.7 Thu 17:15 ZEU 260

An application of the Wang-Landau Monte Carlo method to the modeling of the themal and mechanical behavior of knotted polymer rings in solutions — •Franco- Ferrari[1] and Yani Zhao[2] — [1]CASA* and University of Szczecin, Szczecin, Poland — [2]Centre of New Technologies, University of Warsaw, Warsaw, Poland

The subject of this seminar are the properties and behavior in solutions of single knotted polymer rings. These polymers are defined on a simple cubic lattice. Their statistical properties are investigated by computing the expectation values of a few observables, namely the specific energy, the specific heat capacity and the gyration radius. In the case in which the chain is stretched by a tensile force directed along the z-axis, the average height of the point in which the force has been applied is measured too. The averages are computed exploiting a variant of the Wang-Landau Monte Carlo method. The algorithm has been suitably accelerated and parallelized in such a way that it is possible to sample a large number (from tens to hundreds of billions) of knot conformations. Several types of knots have been considered, including the trefoil, the figure-eight, the cinquefoil knots and many others. From the performed analysis it turns out that knotted polymer rings have a rich variety of different behaviors that can be used in order to tune the properties of polymer materials containing such knots. For instance, these polymers swell faster or slower when heated depending on the type of the knot and on the kind of interactions between the monomers. During the talk some interesting features of the stress relaxation of knotted polymer rings after the stretching force is removed will also be shown.

CPP 60.8 Thu 17:30 ZEU 260

Geometry and topology of periodic filamentous structures — •Myfanwy Evans — Mathematics Institute, TU Berlin, Berlin, Germany

High symmetry dense packings of trees and lines in the two-dimensional hyperbolic plane can be projected to triply-periodic minimal surfaces. The resulting three-dimensional structures are space-filling, symmetric and entangled structures composed of multiple networks or filaments, which challenge current characterisation techniques particularly from the perspective of entanglement. In this talk, I will discuss the construction and characterisation of these complex entangled structures alongside applications from star terpolymer self-assembly to skin swelling.

CPP 60.9 Thu 17:45 ZEU 260

Three-Dimensional Nets from Hyperbolic Tilings — •Benedikt Kolbe — Technische Universität Berlin

A main focus of modern crystallography is to explore the systematic enumeration and construction of nets in Euclidean space. The EPINET project attempts to enumerate crystalline frameworks that arise as structures derived from hyperbolic tilings. Since hyperbolic geometry represents the most prevalent class of geometry not only in nature as a model of the geometry of minimal surfaces, but also mathematically, the use of hyperbolic surfaces to construct possible structures in 3-space is very natural. Among many others, this recipe has also led to deep results in topology from Thurston and others and is also used in modern descriptions of conformal field theory.

We focus on the study of those networks that one encounters typically in the material sciences-periodic structures. Therefore, to classify the emerging structures we employ Delaney Dress combinatorial tiling theory.

We will explain some of the mathematics and intuition involved in a new approach to enumerating the 3-dimensional structures that arise through hyperbolic tilings and give some results on the knotted networks they represent. This work is aimed at generalizing Delaney-Dress tiling theory and to develop a complexity ordering of different tilings.

The most prominent triply periodic minimal surfaces are used to illustrate the approach and provide first examples. The goal of this project is to ultimately construct systematically and order by complexity all networks that arise by decorations of hyperbolic surfaces.