CPP 67: Focus: Topological Problems in the Physics of Polymers, Biopolymers and Fibers II (joint session BP/CPP, organized by CPP)

Time: Friday 10:15–13:00 Location: ZEU 222

CPP 67.1 Fri 10:15 ZEU 222

Mechanical properties of entwined knotted/unknotted DNA loops — •Saeed Najafi and Raffaello Potestio — MPIP, Mainz, Germany

Self-entanglement and knotting can play a crucial role in the mechanical and functional properties of bio-polymers such as DNA and RNA strands and fibers. By means of computer simulations of model DNA systems, we demonstrate that the crossing pattern of a braid of entwined DNA rings has a large impact on its structural and dynamical properties. In particular, we identify under which conditions the braid crossing pattern enforces a positive and stronger correlation between the entangled rings.

CPP 67.2 Fri 10:30 ZEU 222

Entropic interactions between two knots on a semiflexible polymer — •Stefanie Stalter, David Richard, Jonathan Siebert, and Peter Virnau — Institut für Physik, JGU Mainz Staudingerweg 7, 55128 Mainz

Two knots on a string can either be separated or intertwined and may even pass through each other. On the microscopic scale such transitions may occur spontaneously driven by thermal fluctuations and can be associated with a topological free energy barrier. In this manuscript we study the respective location of a trefoil (3_1) and a figure-of-eight (4_1) knot on a semiflexible polymer, which is parameterized to model dsDNA in physiological conditions. Two cases are considered: First, end monomers are grafted to two confining walls of varying distance. Free energy profiles and transition barriers are then compared to a subset of free chains, which contain exactly one 3_1 and one 4_1 knot. For the latter we observe a small preference to form an intertwined state, which can be associated with an effective entropic attraction.

CPP 67.3 Fri 10:45 ZEU 222

Knotted and unknotted ring polymers under shear — •Maximilian Liebetreu and Christos N. Likos — Faculty of Physics, University of Vienna, Austria

The behavior of single 3_1-knotted (trefoil) rings in a fluid under shear is compared to their unknotted ring polymer counterparts. We simulate flexible polymers of a fixed size in a thermostatted Multi-Particle Collision Dynamics (MPCD) solvent (with fixed control parameters) with Lees-Edwards boundary conditions. We primarily investigate the differences in shape parameters for 3_1-knotted and 0_1-unknotted rings in dependency of shear rate, as well as characteristics of average number of beads being part of the knot (knot size), angle between knot center of mass and first principal axis relative to the polymer's center of mass, and correlations between these quantities. We compute the relaxation time of 3_1-knotted rings and present results on their tumbling- and tank-treading dynamics. We obtain evidence suggesting that on a knotted ring, the 3_1 knot itself develops a tendency to be located near those beads closest to the orientational axis, aligned with the flow. We also show that the average knot size is decreasing with increasing shear. Preliminary findings indicate the 3_1-knotted rings responding to lower shear rates than their unknotted counterparts, and suggest a binary-state behavior for the 3_1-knotted ring under strong shear, with the knot size alternating between rather stable tight and relatively unstable delocalised configurations. Special attention is paid to the correlation between alignment angle and knot size.

Invited Talk CPP 67.4 Fri 11:00 ZEU 222

Protein Folding under Mechanical Load — •Matthias Rief — Physikdepartment der TU München, James-Franck-Str. 85748 Garching

The development of nano-mechanical tools like AFM and optical traps has made it possible to address individual biomolecules and study their response to mechanical forces. These techniques allow us to study and induce conformational changes of proteins in real time. In my talk, I will show how single molecule mechanical methods can be used to study folding of proteins. Examples will include the folding of the calcium binding protein calmodulin, as well as the folding of a protein with knotted structure.

15 min break

CPP 67.5 Fri 11:45 ZEU 222

Entropic vs Energetic stiffness in biopolymers — •Tatjana Škrbić[1], Achille Giacometti[1], Trinh Hoang[2], Artem Badasyan[3], and Rudolf Podgornik[4] — [1]University of Venice, Italy — [2]Institute of Physics, Hanoi, Vietnam — [3]University of Nova Gorica, Slovenia — [4]University of Ljubljana, Slovenia

Homopolymers form a high temperature swollen (coil) phase and a low temperature phase globular phase. The glassy nature of this ground state stems from the inability of homopolymers to reduce their entropy as temperature is decreased.

Recent attempts to introduce additional ingredients allowing the removal of this glassy ground state and hence the onset of alpha-helical and beta-sheet like structures, characteristic of proteins, will be presented. In particular, it will be shown how the introduction of an entropic stiffness breaks the spherical symmetry of the interactions and leads to the formation of protein secondary structures.

Further, the difference between this entropic stiffness and the conventional energetic stiffness characteristic of semi-flexible polymers will be pointed out, as well as the relevance of the latter for the ground state phase diagram of DNA in a bad solvent.

Finally, the relevance of the presented results for the protein design, as well as for the interpretation of experimental results on the DNA condensation, will be discussed.

References [1] T. Škrbić et al, J. Chem. Phys. (2016) [2] T. Škrbić et al, Soft Matter (2016) [3] T.X. Hoang et al, Phys. Rev. E (2015) [4] T.X. Hoang et al, J. Chem. Phys. (2014)

Invited Talk CPP 67.6 Fri 12:00 ZEU 222

All-atom simulations of folding of proteins with topologically complex native structures. — •Pietro Faccioli and Silvio a Beccara — Physics Department , Trento University, Trento, Italy

Investigating protein folding using MD remains a formidable task. Using the Anton supercomputer it is now possibile to perform folding simulations of small globular proteins, with folding times in the ms scale. On the other hand, proteins with topologically complex or even knotted native structures can take much longer to fold. Thus investigating these processes by plain MD is well beyond the reach of any present nor foreseen supercomputer.

Our group has developed an enhanced path sampling approach based on a rigorous variational approximation, which enables to simulate the folding of protein of virtually any size with folding time as long as tens of minutes using all atom force fields. This method has been first validated against the results of Anton and then applied to larger systems with increasingly complex topology. In this talk I will review our recent results concerning the folding of the smallest knotted protein and of a serpin, a large (~400 amino-acid) misfold-prone protein with a very complex native structure architecture.

In both cases we find that, in contrast to what happens to simpler globular proteins, sequence-dependent non-native interactions are playing an important role in guiding the folding process, in particular by ensuring that the native contacts are formed in the right order.

30 min panel discussion