Project C1: Conformational transitions of biomacromolecules within ultrathin amphiphilic films

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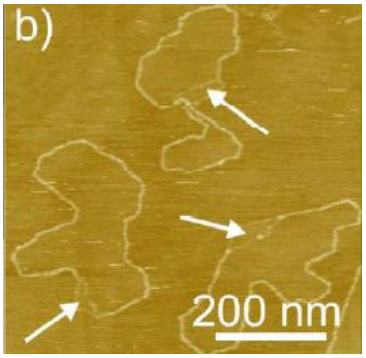
US partner: **Genzer (NCSU)**

Outline. Unwinding and melting a DNA double helical structure at a specific region is the initiation step for DNA replication, with the precise mechanism of it being still an open issue. Experimental and theoretical studies on stretching and twisting of double-stranded (ds-) DNA reveal its chirality by mechanical twist-stretch coupling with small stretching along the DNA backbone inducing torsional stress along the molecular backbone and *vice versa*. It has been theoretically shown that ds-DNA may release its torsional stress inhomogeneously along the backbone with localized, sequence-dependent structural failure to preserve its B-form, when supercoiling is not allowed. Pulling experiments were carried out in solution, where, however, it is difficult to access the direct conformational changes during stretching. Putting plasmid DNA onto or into an ultrathin amphiphilic film wetting the basal plane of graphite allows to overstretch the DNA on the surface. It has been observed that this is associated with local overwinding on the one hand, and local splitting of the double helix into two single strands on the other hand. Only single splits are observed for two different lengths of DNA, with the splitting length being proportional to the total length. A systematic investigation of this process as a function of plasmid lengths, base sequences and the ultrathin liquid film shall be carried out. Taking into account topological considerations it shall be attempted to elucidate the unwinding and splitting mechanism analogue to many biological processes which involve DNA *in vivo* such as replication, transcription initiation, and DNA repair.



Scanning force microscopy image of overstretched vector DNA on a submonolayer of a long chain alkylamine on the basal plane of graphite. The arrows indicate the positions where the double stranded vector DNA split into two single strands.

Research within the German group. The doctoral researcher working on this project shall on the one hand perform the experiments, and on the other hand consider the topological problem, including simple molecular modeling.

Longer-term perspective. Vector DNA is considered as a prototype of a multihelical biopolymer, but multihelices also exist for proteins and other biopolymers. The long-term perspective is to develop a better understanding of the roles of topology and chemical interaction in multihelical biopolymers.

Complementary work in US partner group. In the US partner group it shall be attempted to transfer the process from graphitic substrates to polymeric substrates, which can be stretched macroscopically. This may provide another access to induce conformational transitions in the adsorbed biomacromolecules.

Status of the project. The interaction with the Genzer has been established with the research stay of Liebig during the initial funding period. The project will interact particularly with project A4 (Riegler) on the two-dimensional aggregation of anisometric organic molecules, and A1 (Schoen), where computer simulations will be used to investigate nanostructured molecular systems at interfaces. Changes in the conformation of molecules adsorbed on solid interfaces are also studied theoretically in project A3 (Stark).