Functional molecular films of oligourea-based foldamers

The first part of the project concerns the switchable properties of oligoureas, which fold into a helix, similarly to DNA or alpha-helix of peptides. Such an oligourea folded into a helix is an electric dipole, which is a system of two electric charges at a certain distance from each other. In other words, a dipole possesses a negatively and a positively charged pole. If such a dipole is placed on a positively charged surface, its negative electrical pole will be attracted towards the surface, and the positive dipole will be repulsed from it. In this project we will investigate the conductivity of such helices organised on a gold substrate (electrode) and possessing side functional groups such as carboxylic acid –COOH and amine $–NH_2$ (as in Figure 1). It must be mentioned that oligoureas form more rigid and better bound helices compared to peptides. However, a peptide with these side groups would not fold into a helix.

Depending on the pH (acidity of the solution), the side groups may or may not dissociate. In the acidic conditions the carboxyl group is in its neutral from –COOH, in basic condition it dissociates to $–COO^-$ which is negatively charged. The amine group in basic conditions becomes electrically neutral $–NH_2$ and in acidic conditions becomes a positively charged $–NH_3^+$. As a result, by changing the acidity of the solution, the electrical charges on the helices can be changed. If such helices on a solid substrate, e.g. on gold, are likely charged (f.ex. positively), they will repulse one from another and the solvent will penetrate into the gold interface and the electrode will conduct electricity well. However, if the helices are neutral, the helices will organise into a dense impenetrable layer, the access of the solvent to the gold surface will be hindered and the electric conductivity will decrease. We expect to test the use of such functionalised electrodes as a biocompatible pH sensor.

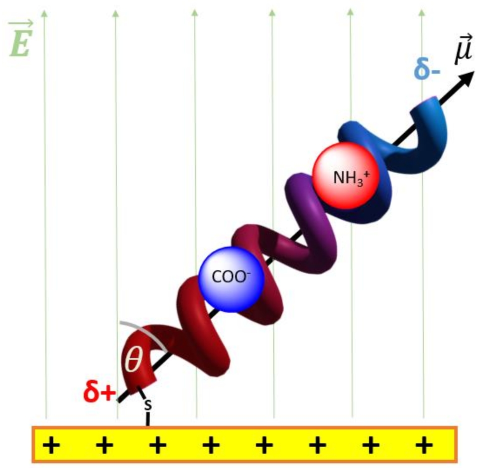

Figure 1 A schematic representation of an oligourea helix with additional charged side groups. The helix is placed in electric field created by the charged surface of the substrate.

The second part of the project concerns biomimetic oligoureas, it is, that try to mimic the structures and processes taking place in nature. Many of the biochemical processes, such as respiration and photosynthesis, involve an electron transfer via proteins, which are large biomolecules composed of several hundred or thousands of amino acids. However, this system is often too complicated to understand the elemental processes taking place there. One could try to isolate a small fragment of the protein where the given process occurs, nevertheless, the structure of a protein is strictly determined by its sequence and such a fragment would fold differently as it is in the protein. In this project we propose an investigation on the electron transfer through oligoureas that fold into helix with similar dimensions and parameters to the alpha-helix in proteins. Moreover, in this project we will investigate the electron transport through oligourea-peptide hybrids. A short peptide chain does not fold into a helix, but when stabilised by a oligourea chain, it forms such a structure. Thanks to this investigation we should gain a better understanding of the processes occurring on short peptide chains.