Hybridization of nucleotide derivatized polydiacetylene monolayer with its complementary mono- and oligonucleotides

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Organic-biological hybrid materials attract much interest in nanotechnology due to the diverse structures and functions of biomolecules and their possible incorporation into nanoscale man-made devices for molecular electronics, nanoelectronics, biological and chemical sensors and their combinations.

We study the formation of nucleotide base-pairs between polydiacetylene (PDA) films derivatized with nucleo-base (10,12 pentacosadiyne cytidyl, PDC) and their complementary mono- and oligonucleotides. PDA films are semiconducting and photoconducting polymers. The electrical properties of conducting polymers are highly dependent on their conformation and electronic configuration. The apparent color-shift of PDA is known to be dependent on structural deformations whose sources include heat, mechanical shear stress, high pH, dehydration and specific binding of biomolecules. In these cases the nature of the structural transition is poorly defined. The small molecular size and regular arrangement of nucleobase-derivatives offer better understanding and allows induction of tailor-made, directed conformational change. The nucleotides moieties pack closely with surface density that is comparable with that of the PDC monomers. The resulting surface presents a dense array of binding sites that are capable of forming base-pairs. The outcome of this recognition is that a new and stable complex of DNA-PDC is formed. For comparison the distance along the helix axis between stacked nucleobases in native DNA is 3.4Å. The discrepancy in molecular distance between nucleobases along a single stranded DNA (5-6.5Å, depending on the strand’s conformation) and the typical π-stack distance in double-stranded DNA helix, is the major cause for the formation of the helix. It is anticipated that nucleotide base-pairs that form at the film interface are π-stacked, as in DNA. This in turn, causes structural deformation that is driven by similar stereochemical considerations as the DNA helix formation.

Elucidation of the structural response of the PDC film upon specific recognition and base-pair formation is the main goal of the proposed project. In this project hybridization of 16G or 8G oligonucleotides on PDC monolayer is investigated by GIXD- grazing incidence x-ray diffraction, BAM- Brewster Angle Microscopy, AFM, TEM, fluorescence measurements,
pressure-area isotherms (on Langmuir film balance) and by Visible Infra Red (Vis-IR) Absorption Spectroscopy.

PDC films are crystalline and diffract grazing incidence x-rays. The hybrid of PDC monolayer with 16G or 8G oligonucleotides enhances the order and longitudinal organization, suggesting long range complementary hybrid structure formation.