Doctoral thesis summary

"Spectroelectrochemical investigations of three dimensional $\pi$-conjugated polymer structures based on 3-alkylthiophenes"

Thesis summary:

The work is focused on the electrochemical, spectroelectrochemical and conductometric investigation of conjugated copolymers that contain 3-hexylthiophene moieties. The three-dimensional molecular architecture was introduced during the design of the studied compounds, by utilising a polysiloxane chain as a scaffold for poly(3-hexylthiophene) (P3HT) chains that were grafted onto it.

During the course of the work, linear P3HT samples were investigated alongside the three-dimensional copolymers, as reference systems, allowing the impact of the transition to the graft architecture to be gauged. Spectroelectrochemical and conductometric methods were used to explore the properties of graft copolymers, containing both P3HT grafts and non-conjugated, poly(ethylene glycol) co-grafts, in order to investigate the effect of grafting density and length of the grafted P3HT chains on the properties of obtained compounds. The impact of changes in the structure of the non-conjugated co-grafts on the properties of the copolymers was also studied.

Analysis of data, acquired by cyclic voltammetry and UV-Vis-NIR spectroelectrochemistry, revealed the existence of polysiloxane segments with different local P3HT grafting densities in the investigated polymer films. In the case of segments with a higher grafting density, crystalline phases are formed, due to the interactions between the neighbouring P3HT chains. Segments exhibiting lower
grafting density, in turn, give rise to the amorphous phase, due to significantly weaker interactions between P3HT chains, which are largely isolated from each other.

The obtained electrochemical, spectroelectrochemical and conductometric results indicate that three-dimensional systems, produced by grafting onto polysiloxane chains, based on P3HT show better properties, in terms of their potential application in photovoltaics and optoelectronics, than their parent systems.

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