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New poly(3-hexylthiophene)-based materials for gas sensors and photovoltaic applications - design and synthesis

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Doctoral thesis

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Abstract in English

The primary objective of this work was design and synthesis of novel class of graft copolymers bearing conjugated polymer followed by molecular characterisation of obtained materials. The subsidiary aim was to preliminary recognise application possibilities of the obtained materials as nitrogen dioxide sensors and in photovoltaic devices.

Copolymer architectures were based on the incorporation into the macromolecule the following segments: poly(3-hexylthiophene) as a model electron-donor conjugated polymer in the field of emerging organic photovoltaics and polysiloxane backbone as inert, flexible, thermally and environmentally stable scaffold for graft copolymers. Series of materials with different co-grafted moieties (such as nonpolar alkyl or polar poly(ethylene glycol)) were employed to tune the morphology and optoelectronic properties of the resulting materials. The structure of parent poly(3-hexylthiophene) and the copolymers was thoroughly evaluated by NMR and FT-IR techniques, additionally supported by molecular weight analysis.

Copolymers bearing co-grafted polyether and alkyl side chains were tested as low-temperature gas sensors for detection of nitrogen dioxide. Copolymers demonstrated higher responses to test gas than pristine poly(3-hexylthiophene). It was demonstrated that especially presence of poly(ethylene glycol) segments improved sensitivity of the sensors. Although dynamics of sensor regeneration at room temperature was slow, it was improved by elevating operating temperature to 50-100°C and irradiation of the working sensor with ultraviolet light.

Copolymers: bearing only poly(3-hexylthiophene)-grafts and the ones bearing co-grafted alkyl chains were tested as bulk heterojunction solar cells with fullerene acceptor. Solar cells based on polysiloxane grafted with poly(3-hexylthiophene) and hexyl chains copolymer demonstrated power conversion efficiencies comparable with poly(3-hexylthiophene)-based device. Moreover, copolymer-based solar cells demonstated higher thermal stability upon prolonged annealing and slightly higher stability upon storing in inert atmosphere compared to poly(3-hexylthiophene)-based devices.

In conclusion, obtained copolymers proved to be promising candidates for the further development of such molecular architectures to fine tune the properties by modifying the structure on the molecular level to obtain materials tailored for highly selective gas sensors and organic solar cells applications.