Synthesis and characterization of physicochemical properties of modified carbon nano-onions - ABSTRACT

Novel systems containing carbon nano-onions (CNOs) were investigated. The CNO surface was covalently functionalized with ferrocene derivatives and non-covalently modified with nickel or zinc hydroxides/oxides. These modifications were aimed to improve both transfer and storage capacity of the electric charge. The increase of photochemical activity and improvement of the electrochemical properties of novel carbon materials provide us with hope ahead of their application in organic photovoltaic cells (OPVs) or energy storage devices such as hybrid batteries.

In the literature section, CNOs were characterized. Structure, synthesis methods, properties and potential applications of these nanoparticles were described. CNOs are spherical structures consisting of hollow fullerene core surrounded by concentric and curved graphene shells with increasing diameters. "Small" CNOs, containing from 6 to 8 carbon layers (c.a. 5-6 nm), have been produced by annealing of nanodiamond at 1650°C in an inert gas atmosphere. CNOs exhibit high thermal and mechanical stability, high reactivity and low toxicity. However, their dispersibility is very low in organic and inorganic solvents. Therefore, a substantial part of literature review was focused on CNO surface and structural modification which in most cases leads to increase their dispersibility along with affects their physicochemical properties. The spherical structure of CNOs allows outer surface modification, without the internal carbon layers damaging. A wide range of potential use of modified CNOs can be expected.

The main aim of research was the covalent and non-covalent modification of the CNO surface, which consequently affects to the improvement of physicochemical and electrochemical properties, such as dispersibility, fotoactivity or specific capacity. The new synthesis routes of novel materials containing CNOs were developed. Composites containing nickel or zinc hydroxides/oxides and CNOs were obtained in three different mass ratios. Also, five acceptor systems involving the covalent functionalized carbon nano-onion surfaces with ferrocene moieties (Fc-CNOs) were synthesized. The composites and derivatives of CNOs were characterized using the following techniques: infrared and Raman spectroscopy, scanning and transmission electron microscopy, X-ray diffraction, thermogravimetric

analysis, the adsorption/desorption of N_2, and electrochemical measurements. Wide range of experimental techniques applied in studies allowed for complex characterization of synthesis materials. Physicochemical properties such as porosity, morphology, chemical composition or electrochemical activity were determined.

The experimental part has been extended to the application study of the CNO composites and Fc-CNOs. The electrochemical measurements involving CNO/$Ni(OH)_2$ and CNO/NiO composites exhibited high values of the specific capacitance up to 1200 $F \cdot g^{-1}$ and long-term cycling stability. Because of excellent capacitance performance of synthesis composites, they can be applied as an electroactive material in hybrid batteries or other energy storage devices. The CNO/ZnO composites and Fc-CNO acceptor systems may have potential use in OPVs, which are promising and very cheap compared to commercially available solar cells. The biggest problem in OPVs, which inhibits the high efficiency of the photovoltaic process, is the assortment of suitable active layer materials. Fullerenes or carbon nanotubes have already been used in OPVs, but their power conversion efficiency (PCE), which is closely related to the energy gap between donor and acceptor, is still too small. CNOs have never been used before in OPVs, which underlines innovation of scientific research. The inverted structure OPVs with CNO derivatives as an acceptor material in the active layer or as an electron transport layer were constructed. The OPVs were characterized by relatively good photovoltaic parameters, with PCE values in the range of 0.83-5.10%.

In conclusion, scientific research was aimed at the synthesis of composite materials containing CNO and hydroxides/oxides of transition metals and acceptor systems of CNOs functionalized with ferrocene derivatives. Application of numerous research methods allowed for complex characterization of the obtained carbon nanostructures. The surface modification of the CNOs led to a change in their physicochemical properties, i.e. an increase in photoactivity and an improvement in the storage capacity of the electric charge. Based on the results, it has been proved that novel materials containing CNOs could be used in energy storage devices and organic solar cells.

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