Poly(3-hexylthiophene) covalently attached to multi-walled carbon nanotubes for electrochemical capacitors

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Composites based on conjugated polymers (CP) and carbon nanotubes (CNT) have been widely explored in electronic devices due to the synergistic effects produced by the combination of these materials¹. The introduction of CP in electrochemical capacitors containing CNT improves the performance because of faradaic processes for energy storage ².

In this work, a chemical route to the attachment of poly(3-hexylthiophene) (P3HT) chains directly onto MWCNTs was carried out. The P3HT-grafted CNT synthesized presented higher connectivity between the two components, which improves the properties and applications. The composite was characterized by FTIR-ATR, H¹NMR, Raman, XPS, TGA, TEM, electrochemical impedance spectroscopy and applied as electrode material in a two-electrode cell of supercapacitor.

Results and Discussion

The reaction followed the steps shown in Figure 1:

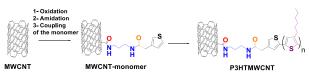


Figure 1. Scheme for formation of the composite.

FTIR spectra of monomer (MWCNT-monomer) and composite (P3HTMWCNT) are presented in Figure 2. The IR spectrum obtained for P3HT showed characteristic bands of the polymer, however, for P3HTMWCNT, were also observed bands that were identified in MWCNT-monomer, as the v(N-H) in 3027 cm⁻¹, v(N-H) and δ (C-N) in 1210 cm⁻¹ and δ (N-H) in 740 and 662 cm⁻¹. XPS spectra showed N1s photoemission peak in 400.5 eV that confirms the presence of an amide carbonyl group; and S2p photoemission peaks in 164.0 and 165.1 eV that are characteristic of P3HT.

Figure 3 shows a) the cyclic voltammograms and b) galvanostatic charge-discharge experiments of the supercapacitor based on composite P3HTMWCNT. It was verified in the voltammograms

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that besides the electric double layer from the MWCNTs, there is a faradaic contribution of the CP, which enhanced the specific capacitance values to attain 311,8 F g^{-1} .

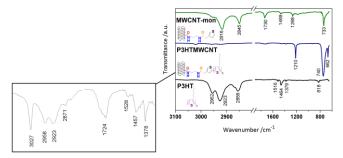


Figure 2. FTIR-ATR spectra of MWCNT-monomer, P3HTMWCNT and P3HT.

Galvanostatic charge-discharge experiments showed a specific capacitance value of 364,2 F g^{-1} and good cyclability up to 3000 cycles.

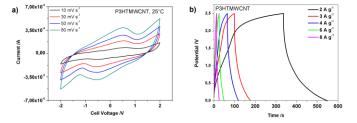


Figure 3. a) Cyclic voltammograms and b) galvanostatic charge-discharge experiments for the P3HTMWCNT supercapacitor using a 0,85 mol L^{-1} LiTFSI/PC as electrolyte.

Conclusions

The physico-chemical characterization confirmed the covalently attachment between MWCNT and P3HT. The application of the composite as electrode in supercapacitor showed promising results.

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¹Fu, C.; et al. *Mater Chem Phys* **2012**, *132*, 596.

²Zhang, H.; et al. *J. Mater. Chem. A* **2014**, *2*, 17024.