

## NOVEL COMPOSITES OF CARBON NANOTUBES WITH A POLY(PHENYLENE ETHYNYLENE) BY NON-COVALENT WRAPPING FOR PHOTOVOLTAIC DEVICES.

Ramos, J.C.<sup>\*1,3</sup>, Cortes, P.<sup>2</sup> Moggio, I.<sup>\*3</sup> Arias, E.<sup>3</sup> Martínez, C.<sup>1</sup> Moreno, K.J.<sup>3</sup>

1. Universidad Autónoma de Ciudad Juárez. Av. del Charro 610, Cd. Juárez, Chih., Méx
2. New Mexico State University. MSC 3805, Las Cruces NM, USA.
3. Centro de Investigación en Química Aplicada. Blvd. Enrique Reyna 140, Saltillo, Coah., Méx, Tel. 01-52-(844)-4389830, Fax. 01-52-(844)4389839. [juankarlosramos@hotmail.com](mailto:juankarlosramos@hotmail.com), [imoggio@ciqua.mx](mailto:imoggio@ciqua.mx).

### Abstract

Conjugated polymers exhibit optoelectronic properties comparable with those of inorganic semiconductors and with the advantage of lower cost of production to recover large areas in thin films from solutions by conventional deposition techniques. These characteristics have opened their application in oLEDs, biosensors and solar cells [1]. By their side, carbon nanotubes (CNTs) offer a great opportunity for exciton dissociation, which is a required factor for photovoltaics, because of their high surface area and different work function comparing with the polymers [2]. For this reason, the combination of conjugated polymer and carbon nanotubes in composites has garnered interest in recent advances for solar cells technology [2]. In this work we present an extensive study on nanocomposites based on a poly(phenylene ethynylene) sequenced with thioester moieties (pPET3OC12-sqS, Figure 1 [3]) with single (SWCNTs) and multiwall (MWCNTs) carbon nanotubes in order to develop novel hybrid materials for photovoltaic cells.

The <sup>1</sup>HNMR analysis suggests  $\pi$  stacking between the rigid conjugated backbone of the polymer and the backbone of the nanotubes on the basis of the high broadening of the phenylene protons peaks in agreement with previous works [4]. This interaction is also reflected in the resonant peaks of both, the thioester-ethyldisulfide and the  $\alpha,\beta$  and  $\gamma$ -O-CH<sub>2</sub>- chains of pPET3OC12-sqS, which practically disappear and likely due to the fact that these spins need more relaxation time to show signals (Figure 1). The absorption and emission maximal wavelengths of the polymer (Figure 2) are maintained when it is wrapped on the nanotubes even if the baseline of the composites UV-Vis spectra is very marked due to the scattering contribution from the nanotubes. The optical band gap decreases in the nanocomposite suggesting an enhancement of the electrical conductivity as confirmed by cyclic voltammetry and by electrical measurement in the films, where the electrical conductivity of the composites resulted one order of magnitude higher than that of pPET3OC12-sqS. A quenching (from 0.55 to 0.49 and 0.27 in the SWCNTs and MWCNTs composites, respectively) of the polymer fluorescence is found, which is attributed to the efficient energy transfer between pPET3OC12-sqS and CNTs, more than the disruption of conjugation by a conformational change as reported in ref. 4 and in agreement with the fact that the absorption and emission maxima are unchanged. Based on these results, the molecular model of Figure 3 was proposed. Micrographs of SEM and TEM microscopy (Figure 4) indicate a good dispersion of the nanotubes in the polymer matrix as well as the absence of bundles of nanotubes in the composite which is consistent with a homogeneous adhesion of the PPS around the carbon nanostructures.

- 1.- Moliton A and Hiorns R.; 2004; Polymer International; 53; 1397-1412.
- 2.- Baibarac M and Gomez-Romero P; 2006; J. Nanosci. Nanotech.; 6; 1-14.
- 3.- Vázquez E. et al.; 2007; Materials Science and Engineering; 27; 787-793.
- 4.- Chen J. et al.; 2002; J. Am. Chem. Soc.; 124; 9034-9035.

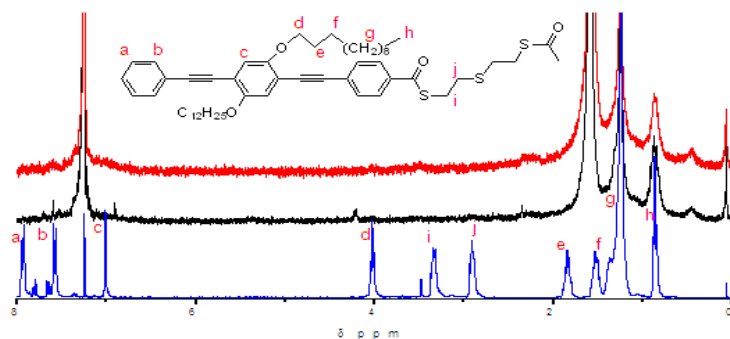


Figure 1.  $^1\text{H}$ NMR spectra of pPET3OC12-sqS (bottom), pPET3OC12-sqS-MWCNTs (middle) and pPET3OC12-sqS-SWCNTs (top). Inserted figure: chemical structure of pPET3OC12-sqS [3].

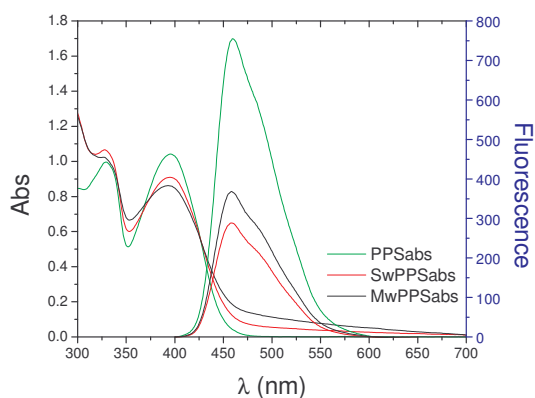


Figure 2. UV and fluorescence spectrum of pPET3OC12-sqS solution and composites suspensions.

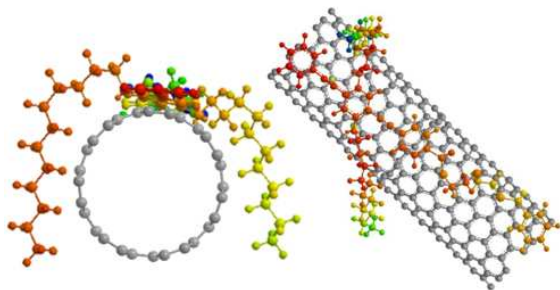


Figure 3. Molecular model proposed for PET3OC12-sqS-CNTs complex.

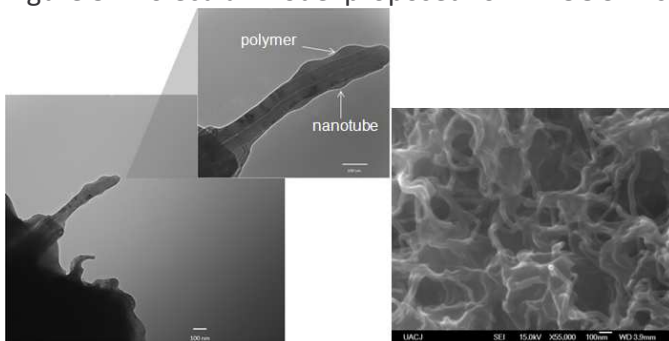


Figure 4. TEM and SEM images of pPET3OC12-sqS-MWCNTs composite.

**Symposium: ADVANCED MATERIALS/ POLYMER NANOTECHNOLOGY**