## P3HT/CdSe/WS<sub>2</sub> Composites for Hybrid Photovoltaics: Structural and Morphological Properties

Amanda Generosi<sup>1</sup>, Marco Guaragno<sup>1</sup>, T. Di Luccio<sup>2</sup>, C. Borriello<sup>2</sup>, A. Bruno<sup>2</sup> and B. Paci<sup>1</sup>

<sup>1</sup>Istituto di Struttura della Materia, CNR Via del Fosso del Cavaliere 100, 00133 Roma, Italy amanda.generosi@ism.cnr.it; marco.guaragno@ism.cnr.it; barbara.paci@ism.cnr.it <sup>2</sup>Centro Ricerche Portici, ENEA Piazzale E. Fermi 1, 80055 Portici, Italy tiziana.diluccio@enea.it; carmela.borriello@enea.it; annalisa.bruno@enea.it

## **Extended Abstract**

Currently, energy demands and concerns on climate change issues are rapidly increasing and much research attention is dedicated to the development of novel strategies to obtain renewable clean energy, photovoltaics being a promising example [1]. In particular, to take advantage of the appealing properties of both organic and inorganic materials, hybrid solar cells (HOSCs) based on conjugated polymers, quantum dots and nanowires are now of great interest. However, to reach attracting electrical performances that are essential to the development of complete HOSCs, the optimization of the architecture and the active materials structural and morphological properties are crucial aspects [2].

In this work, this critical topic is addressed for an original hybrid nanocomposite ternary system based on tungsten disulfide nanotubes ( $WS_2NTs$ ) and cadmium selenide quantum dots (CdSe QDs) embedded into a Poly(3-hexylthiophene-2,5-diyl) (P3HT) polymeric matrix, by means of an unconventional Energy Dispersive X-ray Diffraction technique combined with Atomic Force Microscopy and Raman spectroscopy.

Morphology and structure influence charge transport properties of the composite material[3,4]: not only the energy gap values and the absorption properties of P3HT and WS<sub>2</sub> NTs depend on the polymeric side chains organization and the diameter of the NTs respectively, but performances of the devices could be strongly improved if structural requirements for a directional charge transport are achieved introducing the CdSe QDs. Consequently, a comprehensive understanding of the characteristics of both binary and ternary compounds is critical in order to unveil their possible applications.

This work proved, as a first step, the morphological and structural stability of binary compounds based on  $WS_2$  nanostructures blended into a P3HT matrix. The subsequent addition of CdSe QDs resulted in decoration of the  $WS_2$  NTs and a more homogenous dispersion of the inorganic compounds into the polymeric film was obtained: both results are essential for possible application of this ternary compound in hybrid organic/inorganic photovoltaic cells. Raman spectroscopy supported the crystallographic evidence of CdSe dot configuration and the absence of bulk material that would have been detrimental for application in HOSCs.

Moreover the effect of post deposition  $120^{\circ}$ C thermal annealing was considered. An improvement of the structural properties of the polymeric matrix was observed but most significantly the thermal treatment induced an electronic conversion in WS<sub>2</sub> NTs, detected by Raman spectroscopy. Indeed these nanostructures are essential to mechanically stabilize the organic/inorganic blend, but they also act as charge directional transporters when electronically active and properly decorated with charge collectors as the CdSe dots.

These experimental evidences disclose the structural and morphological properties of CdSe QDs/WS<sub>2</sub>-NTs polymer composites, promoting further development of complete HOSCs based on this ternary system.

## References

- [1] J. Ahmad, K. Bazaka, L. J. Anderson, R. D. White, M. V. Jacob, "Materials and methods for encapsulation of OPV: A review," *Renew. Sust. Energ. Rev.*, vol. 27, pp. 104-117, 2013.
- [2] B. Paci, A. Generosi, D. Bailo, R. Caminiti, R. De Bettignies, V. Rossi Albertini, "Structural/morphological monitoring approach to stability and durability issues of photoactive films for organic solar cells," *Chem. Phys. Lett.*, vol. 504, pp. 216-220, 2011.
- [3] U.Vongsaysy, D. M. Bassani, L. Servant, B. Pavageau, G. Wantz, H. Aziz, "Formulation strategies for optimizing the morphology of polymeric bulk heterojunction organic solar cells: a brief review," *J. Photon. Energy*, vol. 4, pp. 040998 (1-22), 2014.
- [4] S. Sreejith, R. Hansen, H. Joshi, R. G. Kutty, Z. Liu, L. Zheng, J. Yang, Y. Zhao, "Quantum dot decorated aligned carbon nanotube bundles for a performance enhanced photoswitch," *Nanoscale*, vol. 8, pp. 8547-8552, 2016.