

Symposium on **Computing π -Conjugated Compounds (C π C-10)**, Valencia, 1-2. 02.19

SPECTROSCOPIC TECHNIQUES AND DFT CALCULATIONS TO UNDERSTAND CHARGE TRANSPORT MECHANISMS IN OFETs.

Alexandra Harbuzaru,¹ I. Arrechea Marcos,¹ J. T. López Navarrete,¹ R. Ponce Ortiz,¹ M.C. Ruiz Delgado,¹ M. Caironi,² A. Scaccabarozzi²

¹ Department of Physical Chemistry, Malaga University, Malaga, 29071, Spain.

² Center for Nano Science and Technology, Milan, 20129 Italy

E-mail: harbuzaru@uma.es

The organic electronics research field has advanced tremendously in the last decades, but there is still an incomplete understanding of the main mechanisms governing charge injection and transport in such devices. The performance of organic semiconductors is governed not only by their molecular structures but also by their intermolecular assembly in the solid state. Here we use a combination of Raman spectroscopy and charge modulation spectroscopy (CMS) to gather information on molecular and supramolecular levels, of organic semiconductors [1,2] (Figure 1) [3]. This last one is an optical-spectroscopy technique conducted on a real OFETs, that allows us to study *in situ* the charge carriers present at the semiconductor-dielectric interface, where the largest contribution to charge transport occurs. [3]

In this communication we will present the study of the bithiophene imide (BTIn) molecules which exhibit encouraging electron mobilities in OFETs [1,2], by using the spectroscopic techniques presented above, supported by DFT quantum chemical calculations in order to shed light on the mechanism of charge transport in OFETs.

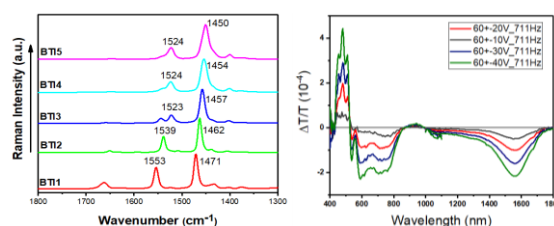


Figure 1: Raman Spectra (left) and CMS Spectra (right).

References

- [1] Y. Yang, H. Guo, S. Ling, I. Arrechea-Marcos, Y. Wang, J. T. López Navarrete, R. Ponce Ortiz, X. Guo, *Angew. Chem. Int. Ed.* 2017, 56, 9924-9929
- [2] Y. Wang, H. Guo, A. Harbuzaru, M. A. Uddin, I. Arrechea-Marcos, S. Ling, J. Yu, Y. Tang, H. Sun, J. T. López Navarrete, R. Ponce Ortiz, H. Y. Woo, X. Guo, *J. Am. Chem. Soc.* 2018, 140, 6095-6108.
- [3] M. Caironi, M. Bird, D. Fazzi, Z. Chen, R Di Pietro, C. Newman, A. Facchetti, H. Sirringhaus, *Adv. Funct. Mater.* 2011, 21, 3371-3381