PUBLISHABLE SUMMARY

The main objective of the "Organic Electronics" project has been the search of new optically-opaque and transparent organic semiconductors, both small molecules and polymeric materials, having excellent processability, ambient stability and electrical properties. These new materials have been tested in Organic Thin Film Transistor (OTFT) architectures. By careful selection of the building blocks, n-type, p-type and ambipolar semiconductors have been achieved with mobilities competing those of the state of the art materials. Furthermore, air stability in organic semiconductors has been greatly improved by insertion of high electro-withdrawing building blocks. The most promising transparent materials have also been tested in transparent TFT structures by using glass substrates and transparent dielectric formulations.

In addition, semiconducting nanostructures with exceptionally large charge carrier mobilities, such as organic nanowires and carbon nanotubes, have been also demonstrated. These nanostructures have been combined with optimized ultra-thin self-assembled dielectrics to afford high-performance and low voltage TFTs. The field-effect mobilities achieved in these novel device structures are among the highest reported in literature.

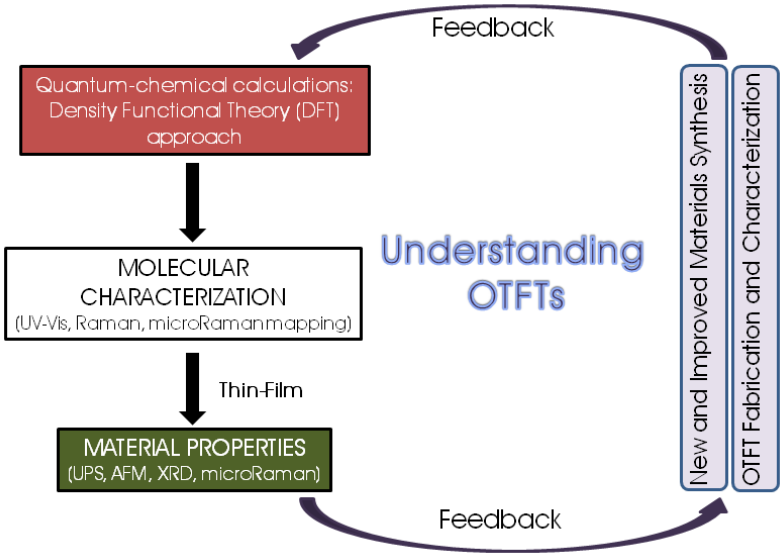
During the whole project, theoretical DFT calculations have been extremely useful to support the experimental results (greatly enhancing the publications quality) and to guide the synthesis of new and improved materials. In fact, during the Return Phase the fellow effort was directed to fully understand, guide and/or improve the semiconductor/dielectric behavior of the materials studied during the Outgoing Phase. Vibrational FT-Raman, microRaman and Resonance Raman spectroscopies were also used to analyze the impact of the semiconductors molecular and electronic properties on the OTFT electrical performance. In some cases, these results afforded the rational design of semiconductors with tailored charge transport in OTFTs. As an example, in one of our projects, by judicious modifications directed by DFT calculations it was possible to modify one inactive semiconductor building block and enhance its electrical performance achieving the synthesis of one of the best n-type polymers published so far. The same approach was used to guide the synthesis of molecular materials for organic photovoltaic (OPV) applications, where the frontier molecular orbitals energetics is crucial in the charge injection/charge dissociation processes.

The results derived from all these projects have been published in 23 articles in high impact peer-review journals.

To summarize it is important to highlight that the approach used during this project (see *Scheme below*) allowed the establishment of molecular/solid state/property relationships with the aim of improving material properties and of guiding both synthetic

chemists and material engineers in the design of new improved molecular materials and device structures.

Scheme indicating the approach used during the "Organic Electronics" Project:



These structure-property relationships are of great technological interest since this knowledge will greatly advance the development of new organic semiconductors and device architectures for environmentally-stable, low-cost and efficient plastic electronics. The information derived from this project can also be extremely useful for other research fields, such as organic photovoltaics. It is widely known that climate change concerns, coupled with high oil prices are driving the development and use of new, and cheap renewable energies. Organic solar cells have appeared as a viable alternative to the current inorganic photovoltaic cells. In this case, the possibility of inexpensive fabrication techniques such as roll-to-roll printing offers the possibility of installing organic solar panels at any location, including stand-alone power stations and on buildings or roads, for developing countries and rural areas, where electrical infrastructure lacks. However, for OPV commercialization it is still mandatory to improve cell efficiency, which is possible following our scientific approach.