

Research Proposal during M. Carmen Ruiz Delgado's Stay at LPPI Lab

The main scope of this research proposal of Dr. M. Carmen Ruiz Delgado in the group of Dr. Gjergji Sini in the LPPI laboratory is to combine vibrational (Raman and IR) and SEM spectroscopic characterization with theoretical DFT calculations to analyze the vibrational and morphological properties of promising organic semiconductors for Dye Sensitized Solar Cell (DSSC) applications. The photovoltaic properties of new p-type amorphous organic semiconductors will be analyzed and compared with Spiro-OMeTAD based control devices.

The Raman technique not only offers the required sensitivity to detect subtle changes in the molecular conjugated backbone, conformation, configuration and micro-domains, but also allows simplicity and non-destructiveness in sample preparation and handling. On the other hand, Scanning electron microscopy (SEM) is a great way to obtain information about a sample's surface topography and composition. Finally, the energy dispersive spectroscopy (EDS) technique will be used to identify and quantify the elements constituents of the sample.

The proposed Raman and SEM studies will help us to analyze in detail the role played by the pore filling properties and dye-sensitized TiO₂/HTM affinity in the photovoltaic performances of obtained devices. Please note that the interfacial hole-transfer yield depends on the extent of pore penetration in the dye-sensitized film and on the thermodynamic driving force for interfacial charge transfer. This implies that the pore filling and interfacial properties are even more important than hole mobility in hole-transport material (HTM) design.

With such an approach, we plan to establish structure/property relationships with the aim to improve the materials properties and to guide synthetic chemists to design new organic semiconducting materials with enhanced performance in DSSCs. The goals proposed in this interdisciplinary research project will be achieved by using a feedback loop: The DSSC materials provided by Dr. Thanh Tuấn Bui and Prof. Fabrice Goubard will be characterized by vibrational and SEM spectroscopic techniques; these experimental data will be further nicely interpreted with the help of quantum-chemical calculations provided by Dr. Gjergji Sini. This research work will provide the candidate the opportunity to collaborate with research groups with complementary expertise, such as synthetic chemists and theoretical chemists, ensuring the success of the proposed objectives in this proposal.