Application of Oligo(ethylene-oxide)-substituted Conjugated Polymers and Small Molecules in Organic Photovoltaic Cells Processed from Green Solvents

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1. Introduction – Photovoltaic devices incorporating soluble organic semiconductors in the photo-active layer represent an attractive route for semi-transparent, flexible, and light-weight solar modules that can be fabricated by low-cost techniques, as roll-to-roll printing. Such advantageous characteristics are due to the properties of organic semiconductors, whose molecular structure can be tailored to afford appropriate opto-electronic properties and good solubility. Recently, photovoltaic devices processed from blend solutions of organic semiconductors have demonstrated high efficiencies (*ca.* 14 %) in small scale laboratory prototypes [1]. Nevertheless, the solvents currently used to process the active layer of state-ofthe-art devices are typically harmful halogenated solvents, such as dichlorobenzene, thus engaging critical issues for transferring the technology to mass production. However, to date there are only a few reports on OPV devices based on organic semiconductors with tailored solubility to "green" solvents, such as water and ethanol. Here, we show a series of new conjugated polymers and small molecules anchoring hydrophilic oligo(ethylene-oxide) solubilizing side chains. Modifications of the molecular design, supported by quantum mechanical methods, allowed to tune the materials 'optical spectra and frontier energy levels (HOMO and LUMO energies) and to establish relevant structure-optoelectronic properties.

3. Results and Discussion – Image 1 shows the general molecular structure of the synthesised materials [2]. The modification of the end unit X allowed to alter both the optical spectra and the HOMO/LUMO energies, such that materials absorbing in the near-infra-red were obtained. Upon combination with electron-donor polymers carrying analogous solubilizing groups, also synthesised by us, the new materials were tested in OPV devices fabricated using different solvents to process the active layer, from conventional/halogenated solvents to "green" formulations, as anisole: ethanol mixtures. The obtained devices´ efficiencies were low but the results allowed to interpret how the solvent affects the morphology of the active layers and the devices´ electrical parameters.

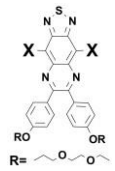

Image 1. General structure of investigated materials.

4. Conclusions – This work provided guidelines for the molecular design and solvent-processing of organic semiconducting materials towards efficient and truly "green" organic photovoltaic devices.

5. References

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