XXXII Panhellenic Conference on Solid State Physics and Materials Science
Conference Center "Carolos Papoulias", 18-21 September 2016, Ioannina, Greece

Chemical structure optimization in high performance electron donor conjugated polymers based on indacenodithiophene and indacenodithienothiophene for organic photovoltaic applications

Athanasios Katsouras, Christos L. Chochos, Apostolos Avgeropoulos
Department of Materials Science Engineering, University of Ioannina Ioannina 45110, Greece

Abstract: Conjugated polymers represent one of the most important class of materials for the fabrication of many optoelectronic applications, such as light emitting diodes, field effect transistors, organic photovoltaics, sensors, etc. In the field of organic photovoltaics, the design of novel conjugated polymers with appropriate frontier orbital energy levels, optical band gap and suitable carrier transport properties are needed to improve the power conversion efficiency (PCE).[1,2] Among various materials developed for bulk heterojunction devices, the multifused-ring conjugated polymers are particularly interesting due to their superior optical and electrical properties.[3] The highly fused aromatic/heteroaromatic units enhance effective conjugation of the polymer backbone to facilitate electron delocalization and charge carrier mobilities.[4] In this work, the design, synthesis and properties characterization of a new family of D-A copolymers based on Indacenodithiophene and Indacenodithienothiophene as the donor units with various electron deficient building blocks (benzothiadiazole, quinoxaline, thienopyrrolodione) will be presented (Figure 1).
In particular, model polymeric semiconductors were designed and successfully synthesized in order to explore, for the first time, the influence of the bond length alternation (BLA) through the polymer backbone enlargement on the optoelectronic properties, as well as the microscopic and macroscopic phenomena.[5] A correlation between structures – properties relationship in this series of model D-A copolymers was achieved. Another important aspect is the role of the polymer's molecular weight. We will report our latest findings on the photovoltaic performance and optoelectronic properties of a donor-acceptor copolymer based on indacenodithieno[3,2-*b*]thiophene and 2,3-bis(3-(octyloxy)phenyl)quinoxaline moieties as a function of the number-average molecular weight (M_n).[6,7] Current-voltage measurements and photo-induced charge carrier extraction by linear increasing voltage (Photo-CELIV) reveal improved charge generation and charge transport properties in these high band gap systems with increasing number average molecular weight, M_n, while polymers with low molecular weight suffer from diminished charge carrier extraction due to low mobility-lifetime ($\mu\tau$) product. By combining Fourier-transform photocurrent spectroscopy (FTPS) with electroluminscence spectroscopy, we demonstrate that increasing M_n reduces the non-radiative recombination losses.
We envision these insights will guide the synthetic chemists and materials scientists towards the optimization of a polymer chemical structure with predetermined optoelectronic properties, controllable supramolecular assemblies and morphologies for specific optoelectronic applications. Therefore, it is evident that the chemistry of functional conjugated polymers is facing major challenges and suitable materials have to adopt a broad range of specifications in order to be established as the best choice for high photovoltaic performance.

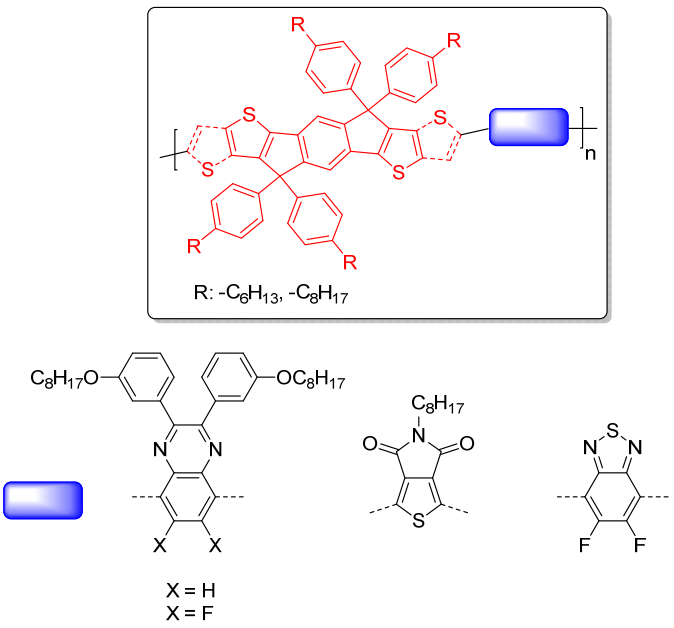

Figure 1: Chemical structures of the indacenodithiophene and indacenodithienothiophene copolymers developed in this work.

Acknowledgment

This project has received partial funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under the Grant Agreement n° 331389 project ECOCHEM

References

[1] G. Li, R. Zhu, Y. Yang *Nature Photon.* **2012**, *6*, 153.
[2] C. L. Chochos, S. A. Choulis, *Prog. Polym. Sci.* **2011**, *36*, 1326.
[3] J. You, L. Dou, Z. Hong, G. Li, Y. Yang, *Prog. Polym. Sci.* **2013**, *38*, 1909.
[4] Y. Li, K. Yao, H.-L. Yip, F.-Z. Ding, Y.-X. Xu, X. Li, Y. Chen, A. K.-Y. Jen *Adv. Funct. Mater.* **2014**, *24*, 3631-3638.
[5] Chochos, C. L.; Singh, R.; Kim, K.; Gasparini, N.; Katsouras, A.; Kulshreshtha, C.; Gregoriou, V. G.; Keivanidis, P. E.; Ameri, T.; Brabec, C. J.; Cho, K.; Avgeropoulos, A. *Adv. Funct. Mater.* **2016**, *26*, 1840-1848.
[6] Katsouras, A.; Gasparini, N.; Koulogiannis, C.; Spanos, M.; Ameri, T.; Brabec, C. J.; Chochos, C. L.; Avgeropoulos A. *Macromol. Rapid Commun.* **2015**, *36*, 1778-1797.
[7] Gasparini, N.; Katsouras, A.; Prodromidis, M. I.; Avgeropoulos, A.; Baran, D.; Salvador, M.; Fladischer, S.; Spiecker, E.; Chochos, C. L.; Ameri, T.; Brabec, C. J. *Adv. Funct. Mater.* **2015**, *25*, 4898-4907.