Studies of charge-carrier transport and trapping in organic solar cells materials

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It is well-known that the problem of charge transport and trapping in organic semiconducting materials has emerged as critical to device performance. The research field of our Kiev group is (i) characterization of defects/traps for charge carriers in conjugated polymers/oligomers, and (ii) a theoretical modeling of charge transport in materials technologically relevant for organic solar cells [1]. We have elaborated and employ extensively an experimental approach based on fractional thermally stimulated luminescence (TSL) and thermally stimulated current (TSC), and have a world-recognized expertise in the application of this method for probing the charge traps and the density-of-states distribution in organic semiconductors.

In particular, we have employed the TSL and TSC techniques for trap characterization in different conjugated polymers as pristine and doped ladder-type poly(*para*-phenylene) (MeLPPP) [2], some substituted PPVs [3], polyfluorene derivatives [4], σ-conjugated polysilylenes [5] and molecularly doped polymers. Using the TSL techniques we were also able to estimate the energy splitting separating the singlet and triplet states of the interchain polaron pairs [6] in conjugated polymers. Recently by combining the TSL and PL-Detected Magnetic Resonance techniques we were able to provide an experimental and theoretical evidence for photogeneration of charged trions in some conjugated polymers [7], a metastable localized quasiparticle consisting of two on-chain polarons of the same sign and a trapped polaron of the opposite sign, which can be metastable with respect to both dissociation and recombination.

Our experimental work is complemented by modeling of the charge transport phenomena. We has recently developed seemingly for the first time self-consistent analytical theory (based on Effective Medium Approach) which is able to account quantitatively for a strongly reduced energetic disorder in some materials [8], effect of positional disorder on negative field dependence of mobility at low fields [9], shallow and deep trapping [4,10], and effects of polaron formation [11] and different carrier densities [12].

The above studies have provided stimulating insights into the electronic structure and dynamics of traps and charge carriers in organic semiconducting materials. Most of the results were obtained in collaboration with other institutes as Philipps-Universität Marburg (Prof. Bässler), Iowa State University (Prof. Shinar), IMEC (Belgium, Arhipov and Heremans), Bergische Universität Wupertal (Prof. Scherf), Eastman Kodak Co. (Dr. Borsenberger), Institute of Macromolecular Chemistry (Prague, Prof. Nešpůrek), etc.

Some selected publications from our group:

1. Book Chapter in ***"Semiconducting Polymers: Chemistry, Physics and Engineering, 2nd Edition"***, Eds. G. Hadziioannou and G.G. Malliaras, (Wiley-VCH Verlag), pp.275-383 (2006).
2. ***Phys. Rev. B.* 63**, 115205 (2001).
3. ***J. Appl. Phys.,* 91**, 5016 (2002).
4. ***Phys. Rev. B.*, 73**, 115210 (2006); ***Chem. Phys,* 291**, 243 (2003); ***J. Appl. Phys.,* 98**, 024101 (2005).
5. ***Phys. Rev. B,* 65**, 165218 (2002); ***Chem. Phys. 234,*** *285 (1998).*
6. ***Phys. Rev. Lett.*, 93**, 066803 (2004).
7. ***Phys. Rev. B*, 76**, 235205 (2007).
8. ***Phys. Rev. B.,* 65**, 125201 (2002).
9. ***Phys. Rev. B.,* 70**, 245212 (2004).
10. ***Phys. Rev. B.,* 66**, 205208 (2002).
11. ***Phys. Rev. B.,* 67**, 224303 (2003).
12. ***Phys. Rev. B.*, 76**, 045210 (2007).