

Conformation of conjugated polymers probed by resonance energy transfer

Short Visit Grant 777

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During my visit to the group of Prof. Arkady Yartsev at the University of Lund (5th to 12th of September 2005) we wanted to measure the femtosecond time-resolved transient absorption anisotropy of poly[3-(2,5-dioctylphenyl)thiophene] (PDOPT). In particular we wanted to investigate that the anisotropy decay is sensitive to the conformation of the macromolecules and subsequently derive this information. Previously we have shown that the depolarisation in conjugated polymer films and solutions is due to excitation energy transfer on disordered polymer chains.¹⁻³

During the visit we were able to record the desired data using a femtosecond absorption spectrometer. Several tests - such as a careful measurement of the power and excitation energy dependence of the femtosecond dynamics - were performed to assure that no other ultrafast process except for exciton energy transfer influences the anisotropy data. We recorded the anisotropy dynamics of PDOPT in good solution (toluene), in poor solution (toluene:ethanol mixture), as a film, embedded in an inert matrix (PMMA) and in decanol, a solvent in which the absorption and emission spectra of PDOPT show a strong temperature dependence.

The experimental data will be the basis for fitting of realistic conformation using a combination of advanced molecular modelling and Monte-Carlo energy transfer simulations. We plan to publish the work in an international peer-reviewed journal. Since we have found an experimental system (PDOPT in decanol) that is suitable for a study of the dynamics of the chain collapse via the temperature dependence we may in future extend the collaboration into this direction.

- (1) Grage, M. M. L.; Pullerits, T.; Ruseckas, A.; Theander, M.; Inganäs, O.; Sundström, V. *Chemical Physics Letters* **2001**, 339, 96.
- (2) M. Grage, Y. Zaushitsyn, A. Yartsev, M. Chachisvilis, V. Sundstrom, T. Pullerits. *Physical Review B* **2003**, 67(20), Art. No. 205207.
- (3) Westenhoff, S.; Daniel, C.; Friend, R. H.; Silva, C.; Sundström, V.; Yartsev, A. *Journal of Chemical Physics* **2005**, 122, art. no. 094903.

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