

# Nanooptics and photonics

## Disorder in P3HT aggregates

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The arrangement of poly(3-hexylthiophene) (P3HT) molecules into ordered crystalline domains is of paramount importance for construction of effective organic solar cells (OSCs), where this polymer serves as a donor material. Inter- and intramolecular ordering of polymer chains is driven by overall structural organization of the P3HT system, including polymer chain regularity, intramolecular conformational changes, intermolecular interaction and packing, which are the crucial factors influencing the photophysics and charge transport in the system. For example, in *regiorandom* P3HT chains the primary excitations are intrachain excitons which give rise to a moderately strong photoluminescence (PL), whereas in *regioregular* chains the excitons are more delocalized through interchain interaction which results in lack of stimulated emission, vanishing intersystem crossing, and very weak PL band [1].

Here, the effect of a solvent on photophysical behavior of polymer chains in P3HT aggregates is reported. P3HT aggregates with the different extent of disorder have been prepared in solutions and thin films cast from the solution, using a combination of good and poor solvents. Electronic absorption and PL spectra evidenced in favor of improved ordering of P3HT chains as a result of use of poor solvents with higher boiling temperature; the ordering was indicated as a decreasing width of Gaussian distribution of molecular transition frequencies. Particularly, formation of H- and J-aggregates in spin-coated films, dependent on the solvent combination or inert polymer matrix used for preparation of the complex films, was concluded. Disorder in P3HT films was analyzed through the ratio of intensity of sidebands to the 0-0 transition in electronic spectra. An increased quantum yield of PL in P3HT aggregates as a result of application of specific solvents for film preparation was found, which is discussed in terms of the reduced torsional disorder of the polymer backbone.

1. Jiang X.M., [Österbacka R.](#), [Korovyanko O.J.](#), An C.P., Horovitz B., [Janssen R.A.J.](#), [Vardeny Z.V.](#) Spectroscopic studies of photoexcitations in regioregular and regiorandom polythiophene films// Adv Funct Mater. -2002.-**12**.-P. 587-597.