

## Conjugated Polymers for Energy Production - DTU Orbit (09/11/2017)

### Conjugated Polymers for Energy Production: Finding Suitable Candidates for Low Cost Solar Cells

This dissertation is aimed at developing materials for flexible, large area, ITO-free polymer solar cells (PSCs) fully printed under ambient conditions. A large screening of conjugated polymers, both novel and well-known materials, has been carried out in order to find suitable candidates for scalable PSCs fully printed under ambient conditions [Adv. Energy Mater. 2015, 5, 1402186]. PPDTBT resulted to be the conjugated polymer with the best photovoltaic performance within the 104 synthesized macromolecules. Therefore, further studies have been done on such material. The impact of side chain position on the physical and electrical properties of PPDTBT backbone have been evaluated, finding that anchoring a branched alkoxy chain to benzene leads to PCE as high as 3.6%, a considerably high performance for flexible ITO-free PSCs (area of approx. 1 cm<sup>2</sup>) [Macromolecules 2015, 48, 3481–3492]. Direct arylation (DAr) and direct arylation polymerization (DArP) have been applied to the preparation of PPDTBT, making this polymer readily available in only 4 synthetic steps and thus easily transferable to a large scale-production setup. DArP avoids organometallic species and therefore is an appealing polymerization method for industrial production of polymers. Several DArP protocols have been employed for the synthesis of PPDTBT leading to polymers with high structural regularity and photovoltaic performances comparable with the same materials synthesized via Stille cross-coupling polymerization. The reactivity of DArP has been further studied and applied to the synthesis of fluorinated copolymers featuring thiophene, which are largely used materials for organic electronics. In particular, by moving the bromine functionality from one monomer to the other, a big impact on the reactivity has been observed. When a thiophene-based donor monomer was brominated and copolymerized with 1,2,4,5-tetrafluorobenzene, hydrodehalogenation side reactions were suppressed, leading to the synthesis of the new PTPf<sub>4</sub> defects-free copolymer [J. Polym. Sci. Part A: Polym. Chem. 2015, 53, 2598–2605].

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