The ECOCHEM proposal is in line with the efforts of the European Union to strengthen low-carbon energy supplies as described in its European Strategic Energy Technology Plan as the Materials Roadmap enabling Low Carbon Energy Technologies (SET-Plan). Today, organic photovoltaic devices (OPV) are known to have the lowest energy payback time. OPV played a minor role until 2013 due to their lower performance (efficiency, lifetime) and the lack of industrial-scale manufacturing of large-area devices. The OPV market follows very optimistic forecasts. Within the market share distribution of different thin film PV technologies, OPV has the potential of becoming the long-term winner. As soon as OPV reaches similar performance levels as the other thin-film photovoltaic technologies (10% module efficiency, 10+ years lifetime), it will enter new markets of large-area applications and building-integrated systems.

The research plan of ECOCHEM targets high quality scientific work combined with technological applications (eg. OPVs) and the obtained results will provide the directions needed to investigate and solve critical issues in order to move an idea from the lab to a prototype and final product. Molecular semiconductor materials and devices have a very crucial advantage compared to traditional inorganic semiconductors: They are easy to handle. They do not require high vacuum equipment. They can be deposited at room temperature from solution, giving hope for low-cost, lightweight, flexible electronics. In addition the new conjugated polymers will expand the implementation of synthesis and preparation for the introduction of several applications, such as for image and lighting, biosensors, organic circuits, etc.

High band gap (HBG) conjugated polymers ($E_g^{opt} \geq 1.7$ eV) with excellent photovoltaic properties, promising environmental stability, and up-scaling ability are highly desirable complementary absorbers for efficient organic tandem solar cells. Contrary to the extensive efforts devoted to the development of low band gap (LBG) donor polymers, the investigation of HBG polymers with suitable photovoltaic properties in inverted architecture solar cells, particularly when processed in air using roll-to-roll compatible printing methods, is barely examined.

Regioregular poly(3-hexylthiophene) (rrP3HT) is the most widely employed high band gap polymer for tandem OPVs due to its reliable photovoltaic performance. The rrP3HT-based solar cells with reasonable performances usually rely on time-consuming device fabrication processes such as thermal treatment and solvent vapor annealing, representing a limiting factor in high-throughput device manufacturing.

In this project new alternating “donor-acceptor” based copolymers have been developed utilizing indacenodithiophene or indacenodithienothiophene as the electron rich monomers and quinoxaline, thienopyrrolodione or difluorobenzothiadiazole as the electron deficient units. The chemical structures of the synthesized copolymers are presented in Figure 1.

All the copolymers exhibit high band gaps similar to rrP3HT. However, the optical properties of the indacenodithiophene and indacenodithienothiophene copolymers are influenced by the choice of the electron deficient unit. When thienopyrrolodione unit is used the band gap of the copolymers is 1.96 eV, whereas when quinoxaline and difluorobenzothiadiazole are used the band gap of the copolymers is 1.79 eV. The energy levels of the indacenodithiophene and indacenodithienothiophene copolymers are shifted to deeper values versus vacuum, as compared to P3HT, and provide better alignment with the energy levels of the [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM). The power conversion efficiency of the unoptimized poly(indacenodithienothiophene–*alt*-quinoxaline) PIDTTQ:PCBM system in inverted configuration (6.1%) is similar to the optimized power conversion efficiency of the rrP3HT based single solar cells demonstrating that PIDTTQ copolymer is an ideal candidate for tandem solar cells as the high band gap copolymer in the front device.

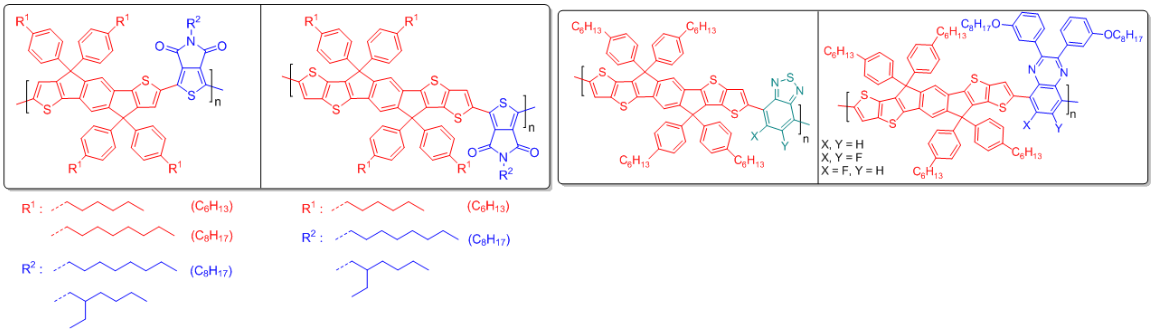

Figure 1. Chemical structures of the synthesized copolymers developed during the duration of ECOCHEM project.

The synthesis of PIDTTQ represents a versatile and reproducible route toward air-processable and efficient high band gap polymers, which could be scaled up for large area processing techniques of single and tandem polymer solar cells. Structure-property relations established in ECOCHEM may contribute to shaping the rational design of high performance semiconducting OPV polymers compatible with roll-2-roll processing techniques. This can be manifested by the demonstration of an OPV flexible module (Figure 2) utilizing the PIDTTQ as the electron donor in the active layer fabricated by one of our colleagues (Department of Materials for Electronics and Energy Technology (i-MEET) University of Erlangen, Germany).

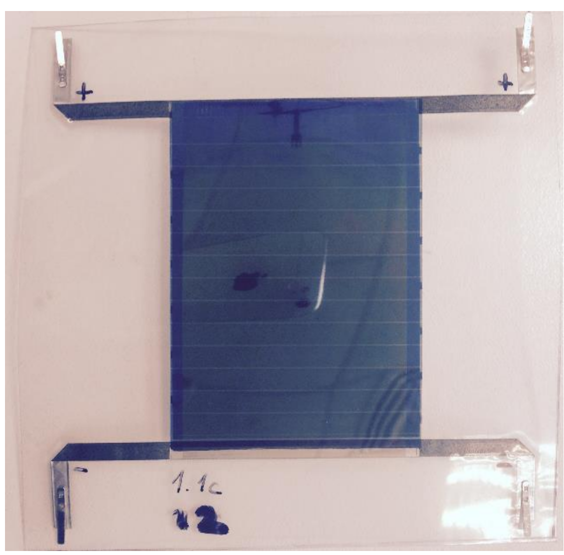

Figure 2. OPV flexible module incorporating the PIDTTQ copolymer in the active layer.