Side Chains with Incompatible Packing: A Strategy to Assemble Organic Semiconductors

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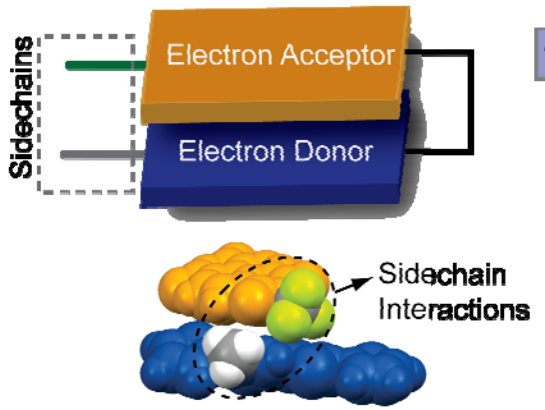
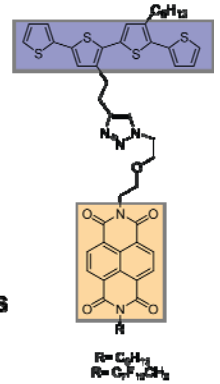
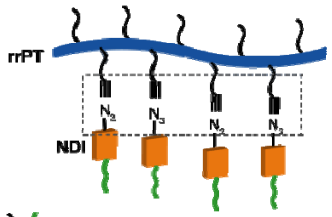
In organic-based photovoltaic cells, it is a challenge to assemble π-conjugated semiconductors, which act as electron- and hole-conductors, into nanoscale structures with a heterojunction between the charge-carrier conductors for efficient charge separation *and* continuous phases of the charge-carrier conductors for high charge mobility. At the present time, blends of organic semiconductors (regioregular poly(3-hexylthiophene) and PCBM) thermally annealed to obtain structures with heterojunctions. However, continued annealing or prolonged use but leads to a precipitous drop in efficiency due to macrophase segregation. Our approach to this problem is to (a) develop chemistry to attach electron conductors to regioregular poly(3-hexylthiophene) (rrP3HT) through covalent or non-covalent interactions and (b) use side chains with incompatible packing to guide the assembly of semiconductors into nanoscale phase segregated structures.

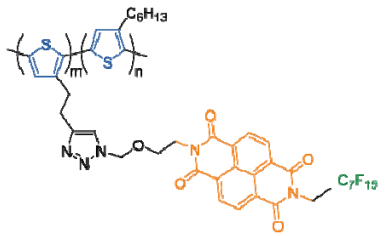
The key accomplishments the ACS PRF grant are:

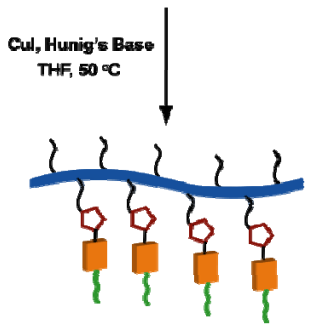
1. Developed and demonstrated the post-polymerization functionalization of regioregular polythiophene by covalently attaching electron conductors and ,
2. Showed in molecular dyads, the sidechains impact the electron transfer rates

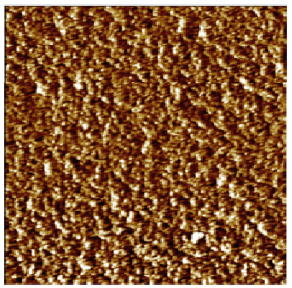












AFM Image of an annealed thin film on Glass showing features of crystalline domains and no macrophase segregation
2 µm x 2 µm