Engineering Band Gap and Energy Levels of Conjugated Polymers for Organic Solar Cells

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The bulk heterojunction (BHJ) organic photovoltaic cells of regioregular poly(3-hexylthiophene) (RR-P3HT) and [6,6]-phenyl C_{61}-butyric acid methyl ester (PCBM) represent one of the most successful systems with reproducible efficiencies approaching 5% after careful optimization. However, with a fixed band gap of 1.9 eV, P3HT can only harvest a small portion of the solar spectrum (maximum 22.4%). In recent years, low band gap polymers for better light harvesting have been intensively pursued. I will review the current status of low band gap polymers. By balancing the open circuit voltage (V_{oc}), the short circuit current (J_{sc}), and the fill factor (*FF*), I will summarize the design criteria for "ideal" polymers to be used in conjugation with PCBM to further improve the efficiency of BHJ photovoltaic devices. A library of novel polymers discovered in my lab with tunable band gap and HOMO/LUMO levels for BHJ organic photovoltaic cells will be discussed in detail to explain these design criteria. A design motif has been proposed, which successfully produced a few polymers that demonstrated close to 5% efficiency in BHJ devices. Detailed studies of these materials help elucidate the structure/properties relationships and provide insights into underlying fundamental transport mechanisms that are essential for intelligent exploration of future organic photovoltaic design.