

Design of Electroactive Materials for Improving Thermal Stability and V_{oc} in Polymer Solar Cells

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We would like to show three different approaches for developing new electroactive polymers to improve the thermal stability of the BHJ solar cells, which is a critical problem for the commercialization of these solar cells. In the second part of talk, we will discuss the development of electroactive materials for improving the open circuit voltage (VOC) in polymer solar cells. The ability to tune the LUMO/HOMO levels of electroactive materials in active layer of polymer solar cells is critical in controlling their optical and electrochemical properties because the HOMO and LUMO offsets between the polymer donor and the electron acceptor strongly affect charge separation and the open circuit voltage (VOC) of a solar cell. First, we enable facile control over the number of solubilizing groups ultimately tethered to the fullerene by tuning the molar ratio between reactants from 1:1 to 1:3, thus producing *o*-xylenyl C60 mono-, bis-, and tris-adducts (OXCMA, OXCBA, and OXCTA) as electron acceptors with different LUMO levels. Second, we present a series of novel poly[3-(4-*n*-octyl)phenylthiophene] (POPT) derivatives (POPT, POPTT, and POTQT) as electron donors with different side-chain density.