

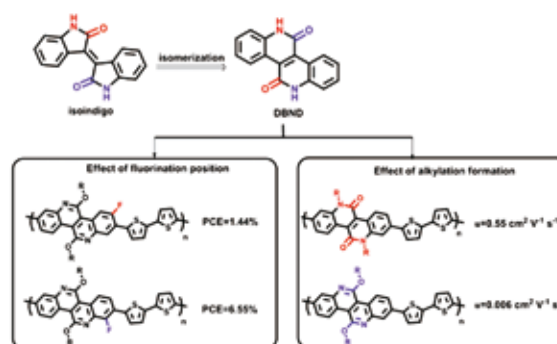
Toward Making Better Organic Semiconductors

Organic conjugated polymers have attracted considerable attention from all over the world in the prospect of producing highly efficient, large area, and flexible organic electronics with tunable properties. The potential applications of organic semiconductors include organic field-effect transistors (OFETs), organic bulk heterojunction organic solar cells (OPVs), organic light emitting diodes (OLEDs) and organic sensors, etc. However, the conjugated polymers with ultra-wide bandgap ($E_g > 2.2\text{eV}$) have exhibited very low power conversion efficiency.

Recently, a research team led WAN Xiaobo from the Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences in Qingdao declared to have synthesized a novel conjugated polymer with ultra-wide band gap, which displayed a high efficiency in converting sun light into electricity and exhibited a very interesting charge transfer behavior.

This novel polymer is based on a key lactam acceptor building block called dibenzonaphthyridinedione (DBND), which can be synthesized via the isomerization of isoindigo, a well-known pigment. They found conjugated polymers based on O-alkylated DBND exhibited photoelectric conversion efficiency (PCE) up to 6.32%. Such a high PCE was obtained without additives or annealing process, which showed little decay in a thicker active layer and little sensitivity to the weight ratios of active ingredients. These merits make DBND based polymer a potential material for processable large-area tandem or ternary OPVs.

They also discovered that such a wonderful performance was strongly influenced by the backbone fluorination positions. OPV devices based on *para*-fluorinated DBND polymers showed best PCEs up to 6.55%, while those based on *ortho*-fluorinated polymers only exhibited PCEs less than 2%, though both polymers have the same bandgap, similar HOMO/



Structure of DBND and the corresponding polymers.

LUMO energy levels and torsion angle. These results suggested that the control of fluorination positions on the polymeric backbone may have a profound influence on the outcome of the OSC performance, which should be paid more attention to for the future design of conjugated polymers for better OSC devices.

More interestingly, they found that the change of the alkylation positions on DBND had strongly influenced the charge carrier mobility of the corresponding polymers. Although with the side-chain branching point one atom closer to the main chain, N-alkylated DBND polymer showed much higher hole mobility ($0.55\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$), almost 100 times greater than that of O-alkylated isomer. It indicated that the major difference between N-alkylated and O-alkylated conjugated polymers lies in their different polarity, in which higher polarity favors tighter interchain packing, which overwhelms the lower steric hindrance of O-alkylation.

Their work shed lights on the structure-property relationship of conjugated polymers, and might be helpful for the design of novel lactam-containing conjugated polymers in the future. The studies were supported by the National Natural Science Foundation of China.