論 文 の 要 旨

題　目 Design and Synthesis of Naphthobisthiadiazole-based Semiconducting Polymers for Non-Fullerene Organic Photovoltaics

（非フラーレン型有機太陽電池に向けたナフトビスチアジアゾール系ポリマーの開発）

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π-Conjugated polymers, also called semiconducting polymers, have been attracted considerable attention due to the solution-processability and excellent electronic properties. Such interesting features allow us to apply them as semiconducting materials for organic electronics devices. One of the devices that are most strongly reliant on the properties of semiconducting polymers is organic photovoltaics, in which the semiconducting polymers are typically used as the p-type material in combination with fullerene derivatives or non-fullerene acceptor as n-type materials. Our group has been focusing on a series of semiconducting polymers based on naphthobisthiadiazole (NTz), which have shown power conversion efficiencies (PCEs) of more than 10% in combination with fullerene materials as the acceptor, which is among the highest values for fullerene-based cells. With this in mind, I envisioned that use of NTz-based semiconducting polymers in the photovoltaic cells in combination with emerging non-fullerene acceptors can provide further high PCEs.

In this dissertation, I designed and synthesized two series of NTz-based semiconducting polymers through different polymer design strategy, named BDT-NTz polymers and NTz-TPTz random copolymers. In the first project, I will show that BDT-NTz polymers exhibited better solubility due to the suppressed polymer crystallinity and weaker sidechain interdigitation than that of PNTz4T, which may afford more well-mixed donor/acceptor blend films that are effective for increasing the photocurrent. BDT-NTz polymers also had deeper HOMO energy levels than PNTz4T, which is beneficial for improving the photovoltage. In the second project, I will show that the NTz-TPTz random copolymers gave significantly higher solubility even by adding small amount of TPTz core unit (2.5~10%) into the PNTz4T backbone. Interestingly, NTz-TPTz was found to have face-on backbone orientation that is favorable for photovoltaic cells while PNTz4T had edge-on orientation. Consequently, we obtained a PCEs of around 13% for BDT-NTz polymers and around 11% for the NTz-TPTz random copolymers. We will discuss the structure–property relationship of the polymers in comparison with PNTz4T in details.