Microcrystal Electron Diffraction for Molecular Design of Functional Non-Fullerene Acceptor Structures

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Non-fullerene acceptors (NFAs) have revolutionized the field of organic photovoltaics (OPV). As a result, devices made from NFAs have begun to reach unprecedented power conversion efficiencies of more than 18%, compared to OPV devices made with fullerene derivatives which stagnated at ca. 11%. The success of fullerene derivatives can be partly attributed to the isotropic charge transport that results from their spherical shape. However, the relationship between molecular structure, solid-state organization and optoelectronic properties of NFAs requires further study. Determining the atomic structure of NFAs and many other solution-processable organic semiconductor (OSC) materials by traditional methods such as X-ray crystallography remains very difficult.

In this talk, I will discuss how microcrystal electron diffraction (MicroED) has helped to advance our understanding of the effects of molecular structure on the solid-state optoelectronic properties of NFAs. Using MicroED, we were able to determine the atomic structures of two well-known NFAs: o-IDTBR and ITIC-Th. Notably, the structure of o-IDTBR was determined from a commercially available powder without the need for additional crystallization steps. The MicroED structure of ITIC-Th is a previously unknown polymorph, with the most distorted backbone of any NFA. Electronic structure calculations based on our MicroED results allow us to shed light on the impact of molecular structure, packing and lattice topology on charge transport in NFAs.

MicroED is becoming an important tool in many areas of chemistry and materials science, and it has the potential to help us more easily elucidate the relationship between molecular structure, atomic structure and OPV device performance.