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Harvesting energy from sunlight directly using solar cell technology is considered as being one of the most important ways to address growing global energy needs using a renewable resource. Organic solar cell (OSC) is the one alternative for producing clean and renewable energy because it can be fabricated onto large areas of light-weight flexible substrates by solution processing at a low cost. Thus, an important research area is the development of new materials for solar cells. Ideally these materials will lead to devices which are cheaper to fabricate and require less energy to produce than silicon solar cells. Possible alternatives to silicon solar cells include semiconductor thin films, the dye sensitized solar cell (DSSC), and thin films of organic materials such as \( \pi \)-conjugated polymers, oligomers, or small molecules.

To improve the OSC performance, the author focuses on the molecular design, synthesis and characterization of DPP-based electron-donating small molecules and oligomers for efficient solution-processed organic solar cells. Our intention here is to utilize self-organization of liquid-crystalline (LC) characteristics and high absorption capability of acceptor/donor/acceptor (A-D-A) type molecules for the fabrication of bulk hetero-junction (BHJ) structures in OSCs, for achieving high photovoltaic performance.

In Chapter 1, a general introduction of the solar cells is presented. Based on this background, the motivation for this research is explained and new molecules for efficient solution-processed OSCs are proposed.

In chapter 2, self-organization of liquid-crystalline (LC) molecules is utilized for the fabrication of well-ordered BHJ architectures in small-molecule OSCs. For the small-molecular system, the important advantages are monodispersity and well-defined structure, easy purification, and less batch-to-batch variation (better reproducibility), but the main problems are inferior film quality and interconnectivity in the active layer due to their intrinsic crystalline nature, which results in low device fill factors. If the scale of the phase-segregated domains in the BHJ layer is smaller than the Coulomb capture radius, it will increase the geminate or bimolecular recombination probability. Therefore, the self-organizing LC DPP-based donor molecules (DPP-TP6 and DPP-TP12) with low bandgap and deep HOMO energy level are synthesized and characterized. DPP-TP6 showed liquid crystalline property, and thus inter molecular orientation can be controlled through thermal annealing. The short circuit current density \( J_{sc} \) and fill factor (FF) values have increased significantly for the DPP-TP6-based devices through the LC organization process.

In Chapter 3, to further enhance the photovoltaic properties, A-\( \pi \)-D-\( \pi \)-A long \( \pi \)-extended narrow-bandgap oligomers, BDT-DPP, IDT-DPP, and T-DPP, having high absorption coefficient are designed and applied to BHJ structures in OSCs. In addition, the impacts of these different central cores on their photophysical and morphological properties, carrier mobility, and photovoltaic performance are
investigated. For oligomeric system, limited photovoltaic performance factor is a relatively low current density, which is partially due to a poor spectral overlap between the absorption of the active layer and solar irradiation. Therefore, spectral overlap between solar spectrum and absorption range of the electron donor material is very important factor for enhancing the efficiency. The design of A-π-D-π-A structures enable to further lower the optical band gap, by interconnecting electron-donating unit with electron-deficient units, as a result of the strong donor-acceptor ICT. To improve the device performance, the effects of additive on photovoltaic performance are also investigated, in which the molecular packing and film surface morphologies are strongly affected by the central donor units. The $J_{sc}$ and FF values can increase significantly for the BDT-DPP-based devices with use of an additive.

Finally, the research is summarized in Chapter 4.