有機薄膜太陽電池のドナー／アクセプター界面における ポリマー鎖垂直配向の影響

Effects of End-on Orientation of Polymer Chains at Donor/Acceptor Interface on Organic Photovoltaic Performance

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The efficiency of charge generation and recombination at a donor/acceptor (D/A) interface of organic photovoltaic (OPV) strongly depends on the interfacial molecular orientation of donor and acceptor materials. Edge-on (i.e. the main chain is parallel and the π-plane is perpendicular to D/A interface) and face-on (i.e. both the main chain and π-plane are parallel to D/A interface) orientations was obtained for the same π-conjugated semiconducting material at D/A interface by proper solvent selection.[1] Several studies have been performed to clarify the effects of these orientation difference on OPV performance. Recently, we reported the formation of end-on orientation (i.e. the main chain is aligned vertical to the surface).[2-3] This is based on the formation of surface segregated monolayer (SSM) of P3BT-F_{17} on P3HT film (Fig. 1a). For the end-on orientation, strong electronic and optical anisotropy and unique photophysical behavior were observed. [2-3]

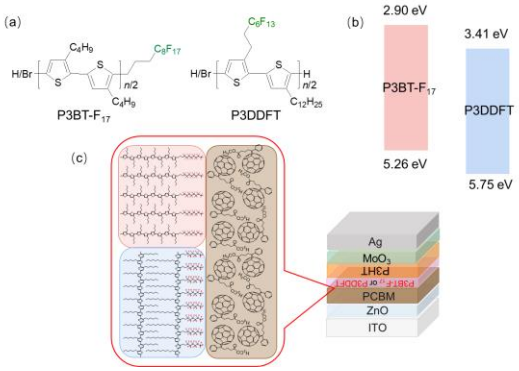

Fig. 1 (a) Chemical structures of materials used in this study. (b) Energy levels of P3HT/P3BT-F_{17} and P3HT/P3DDFT. (c) Schematic illustration of bilayer devices with end-on and edge-on orientation at D/A interface.

In this study, P3BT-F_{17} and P3DDFT (Fig. 1a) were utilized to form SSMs on top of P3HT with the end-on and the edge-on orientation on the surface, respectively. Ultraviolet photoelectron spectroscopy (UPS) and low energy inverse photoelectron spectroscopy (LEIPS) were performed on P3HT/P3BT-F_{17} and P3HT/P3DDFT films to evaluate the energy levels. As the result, rigid energetic shift of ~0.5 eV was observed, indicating the change of electronic structure of film surface influenced by molecular quadrupole moments (Fig. 1b). By contact film transfer (CFT) method[4], bilayer OPVs with the architecture of ITO/ZnO/PCBM//P3BT-F_{17} and P3DDFT/P3HT/MoO_3/Ag were fabricated with the end-on and the edge-on orientations at D/A interface, respectively (Fig. 1c). We found that the end-on device showed improved charge separation and suppressed charge recombination compared to the edge-on device. These may be attributed to the vertical orientation of the main chain that affects the interfacial charge transfer state through the charge delocalization direction.

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