Impact of Dipolar Molecules on OPV Reliability

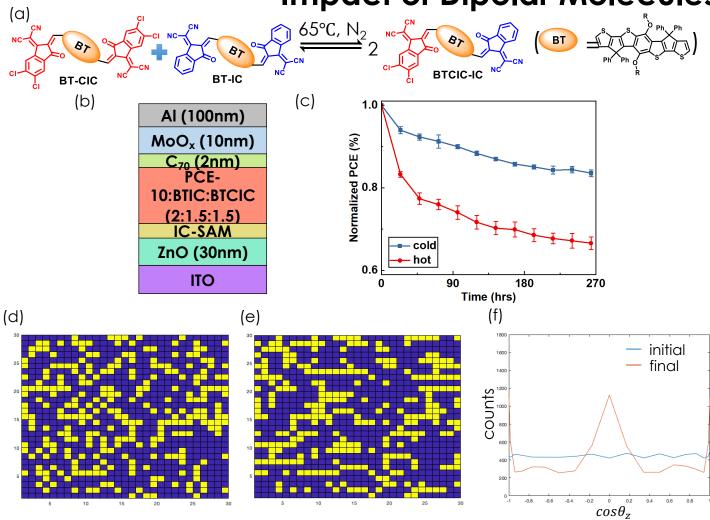


Figure: (a) Schematic illustration of chemical reaction happened between nonfullerene acceptors which results in dipolar molecules reaction products. (b) Illustration of device stack structure. (c) Degradation in power conversion efficiency (PCE) of cold **Contact** (w/o chemical reaction) and hot (w/ dipolar product) ternary devices. Preliminary simulation results of distribution of dipolar molecules in (d) fresh devices and (e) aged devices, the yellow positions are occupied by dipolar molecules, whereas the blue positions are occupied by non-dipolar ones. (f) Simulation results of dipole moments orientations before and after aging.

Objective

> To understand the impact of dipolar molecules re-orientation on the electric field in OPV devices and hence the charge extraction efficiency and reliability of devices

Impact

Ternary blend organic photovoltaics (OPVs) comprising one donor and two non-fullerene acceptors (NFAs) have shown substantial increase in power conversion efficiency over the last decades. Our research reveals that chemical reactions would happen during the fabrication of such devices, which will result in the emergence of dipolar molecules in the ternary blends and leads to reduced device stability. Here, we investigate the re-orientation of dipolar molecules during device aging due to dipole-dipole interaction. The orientation of the dipole moments would tend to be anti-parallel with their neighbors and the dipolar molecules would agaregate during device aging. These changes can affect the electric field across the bulk heterojunction, and hence the performance of OPV devices after aging.

Facilities and Methods Used

- Vacuum thermal evaporation
- Spin-coater

Funding

- US Department of Energy, Solar Energy Technologies Office,
- US Office of Naval Research
- Universal Display Corporation

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