Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Enhanced performance in isoindigo based organic small molecules field effect transistors through solvent additives

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1. Output characteristics of isoindigo based small molecule FETs

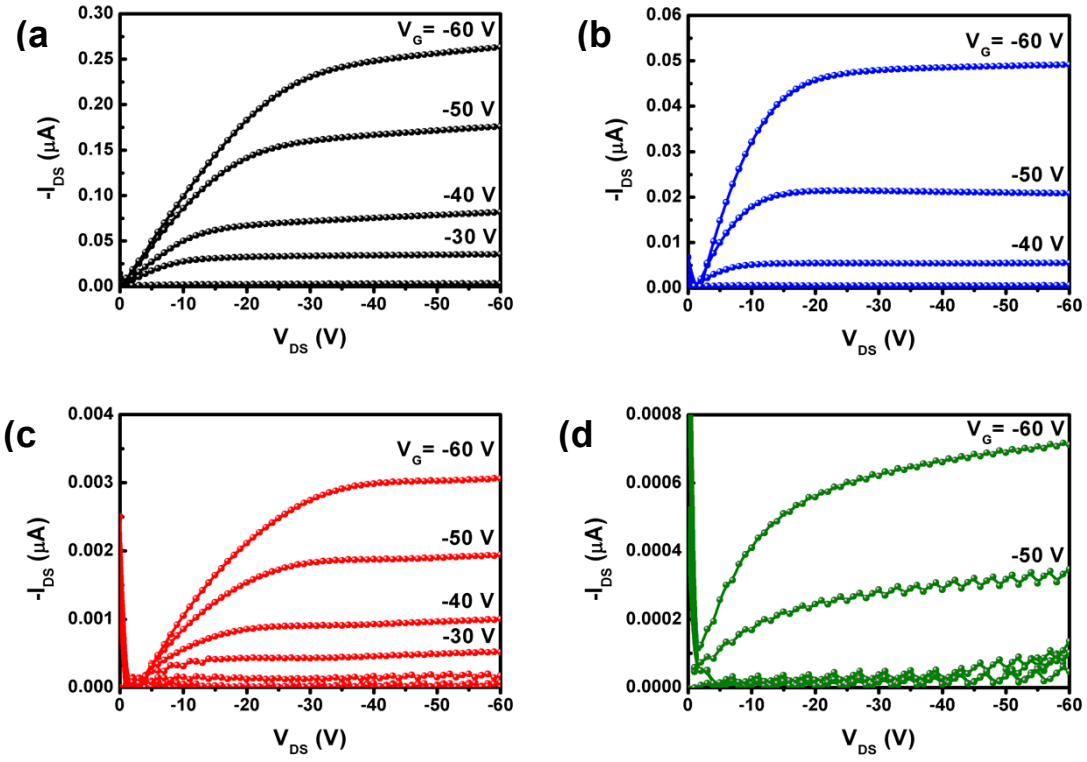


Fig. S1 The best output characteristics of the FETs; (a) IDT with 0.2%, (b) ID2T with 0.2%, (c) ID3T with 0.2% and (d) IDED with 0.5% DIO.

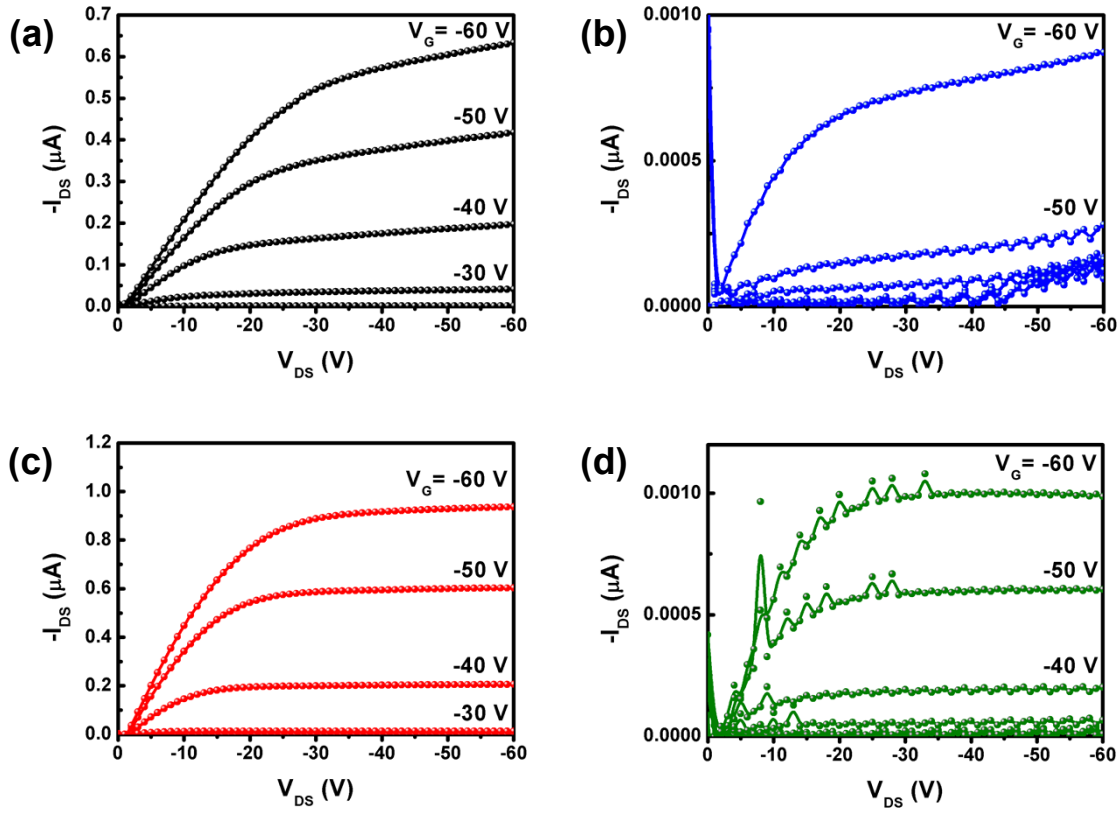


Fig. S2 The best output characteristics of the FETs; (a) IDT with 0.5%, (b) ID2T with 0.2%, (c) ID3T with 0.2% and (d) IDED with 1% CN.

2. UV-vis spectroscopy

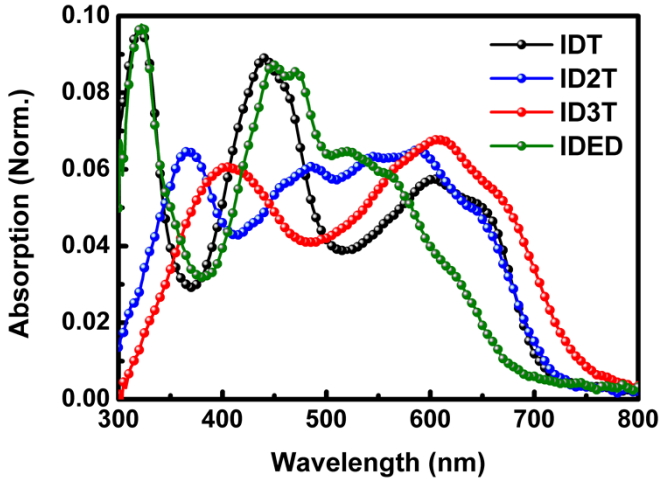
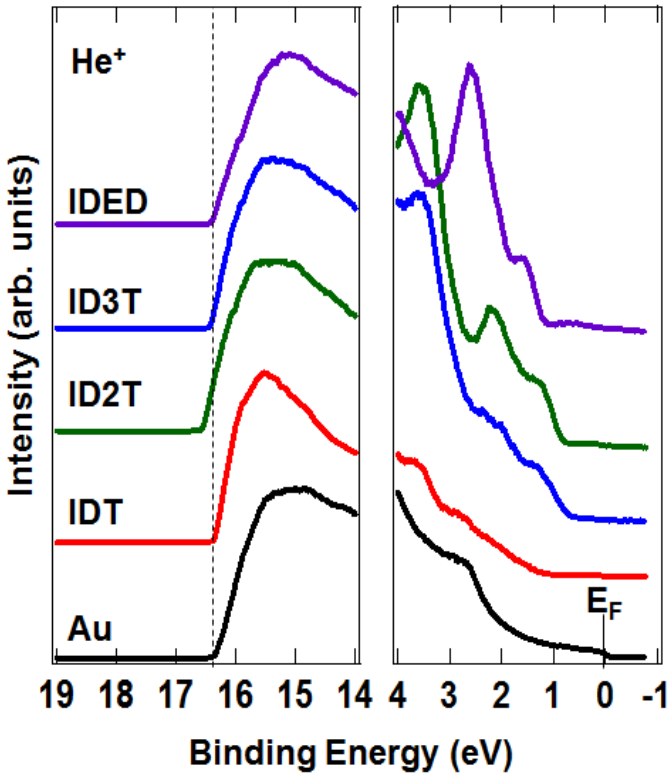


Fig. S3 UV-vis absorption spectrum of isoindigo small molecules.

UV-vis spectra are in general agreement with spectra previously reported for this series of materials, showing similar absorption maxima with small differences in the intensity of shoulder features, which we attribute to subtle differences in environmental conditions in each laboratory during film fabrication.

3. Ultraviolet photoelectron spectroscopy (UPS)

Figure S4 displays the UPS spectra of isoindigo small molecules and Au as a reference. The right-side of Fig. S4 shows the HOMO onsets of isoindigo small molecules. The HOMO onsets of ID2T and ID3T shift toward lower binding energies relative to that of IDT. This indicates that the HOMO energy is decreased as a function of increase of thiophene number as the donor moiety. The HOMO levels of IDT, ID2T, ID3T and IDED are - 6.15, - 5.70, -



5.52 and - 6.03 eV, respectively.

Fig. S4 UPS spectrum of isoindigo small molecules.

4. Density functional theory (DFT) calculations

We performed density functional theory (DFT) calculations at the B3LYP/6-31G level using Gaussian 03 program in order to understand the electrical properties of isoindigo based small molecules. Figure S5 shows the charge-densities isosurfaces of the HOMO and LUMO levels of IDT, ID2T, ID3T and IDED. The charge-densities of the HOMO are generally delocalized on isoindigo based small molecules. In contrast, those of the LUMO are localized along the isoindigo backbone partially. Energy levels of isoindigo small molecules are summarized in Table S1.

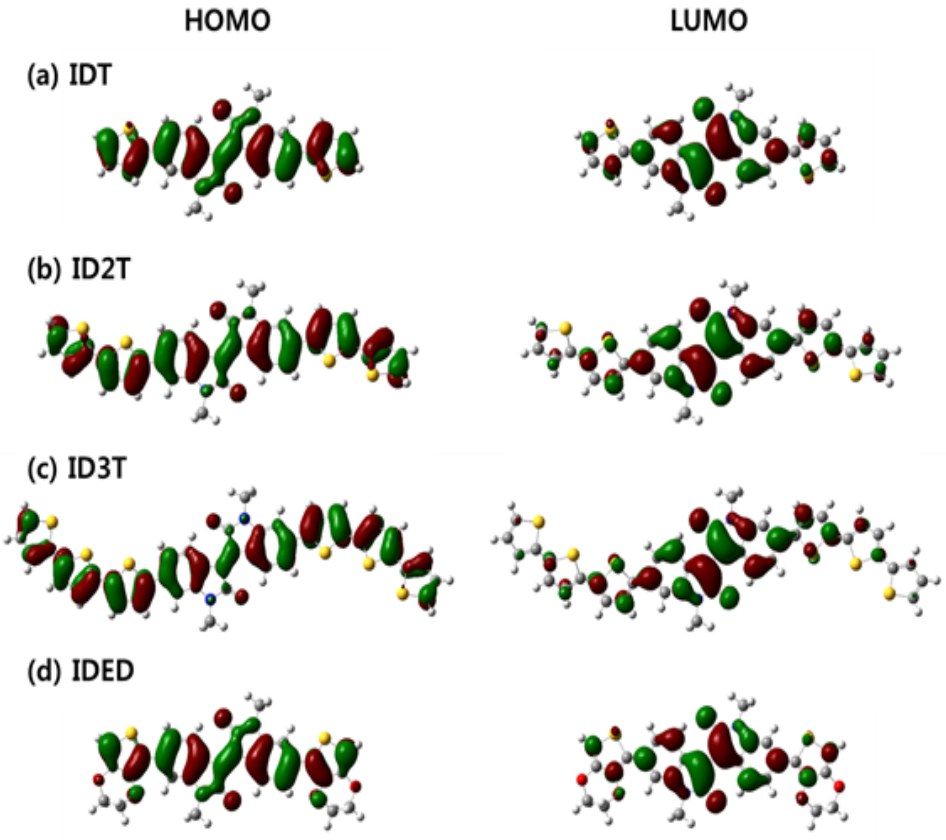


Fig. S5 Charge-densities isosurfaces of the HOMO and LUMO levels of (a) IDT, (b) ID2T, (c) ID3T and (d) IDED.

5. Energy levels

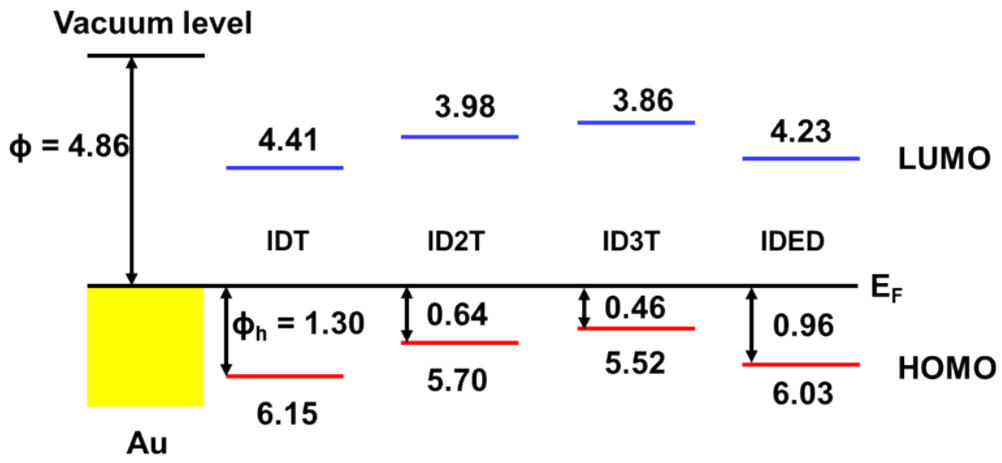


Fig. S6 (a) Energy levels of isoindigo small molecules.

6. XRD diffraction pattern

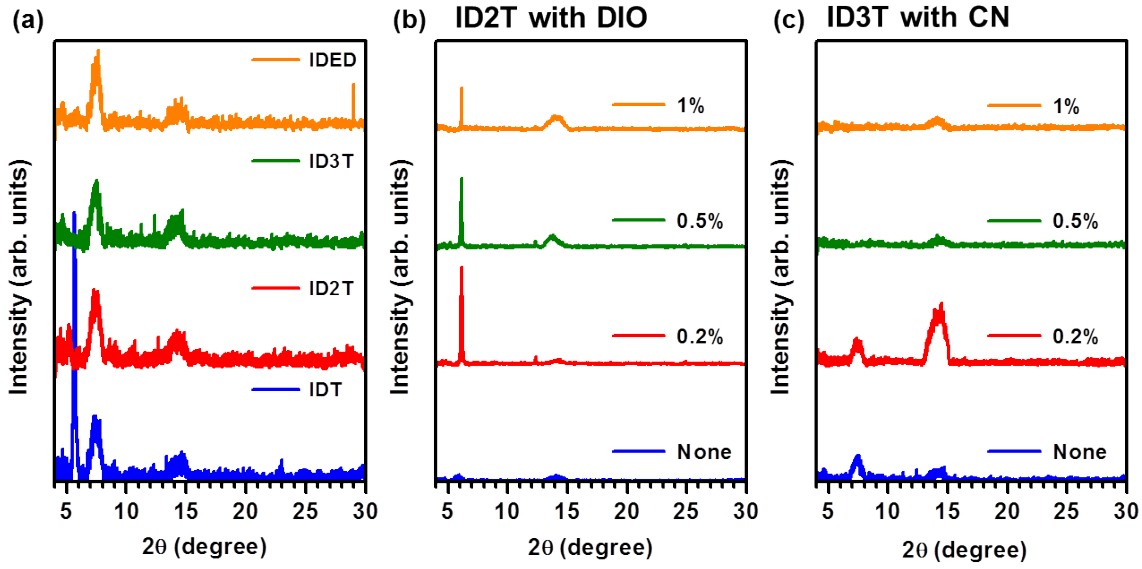


Fig. S7 XRD diffraction patterns of (a) four pristine isoindigo, (b) ID2T films with DIO and (c) ID3T films with CN as a function of concentrations.