*Supporting Information*

# High performance n-channel organic thin film transistor based on naphthalene diimide

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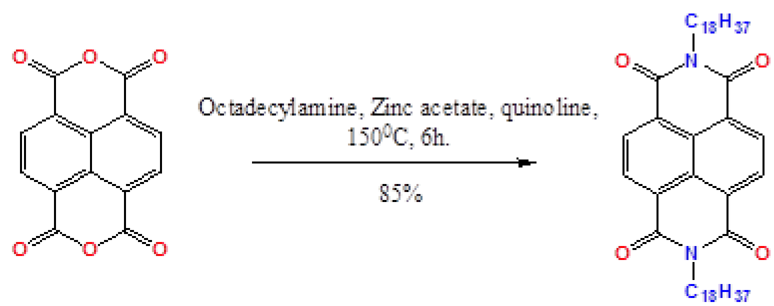



**Figure S1**: Synthesis of NDI-OD2

NDI-OD2 was synthesized by direct condensation of naphthalene dianhydride with octadecylamine. A mixture of 1, 4, 5, 8-naphthalenetetracarboxylic acid anhydride (0.5 g, 1.8 mmol), octadecylamine (3g, 11.16 mmol), and zinc acetate (25 mg) in 15 mL quinoline was heated at 150 °C for six hours. The mixture was cooled and diluted with several volumes of methanol. The resulting slurry was filtered; the collected solid washed with methanol and dried in air. The crude product was then purified by column chromatography using hexane-chloroform as eluent. (Yield: 85%). $^{1}$**H NMR** (400 MHz, $CDCl_3$) δ (ppm): 8.76 (s, 4H), 4.17 (t, 4H), 1.72 (m, 4H), 1.22 (m, 60H), 0.93 (t, 6H) ppm.$^{13}$**C NMR** (100 MHz, $CDCl_3$) δ (ppm):163.03, 131.12, 129.00, 126.97, 41.21, 32.13, 29.90, 29.57, 28.29, 27.29, 23.19, 14.32. **FT-IR** (KBr, $cm^{-1}$, $\nu$): 2921, 2847, 1707, 1657, 1338, 1246, 766.

## Gaussian Calculation:

Software used= Gaussian 03
Basis set used= B3LYP/6-31G (d)

**Molecule:**

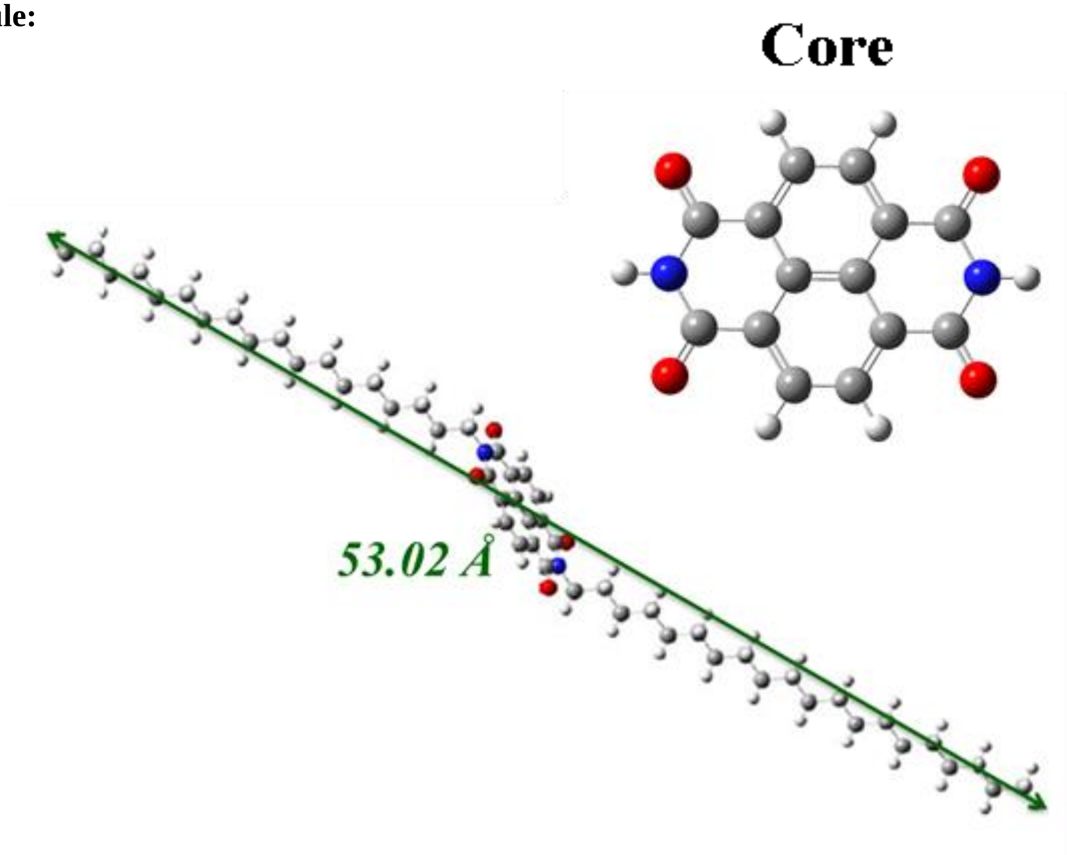



**Figure S2.** The molecular structure of NDI-OD2.

**DFT Calculation Data:**

| | | | | | |
|---|---|---|---|---|---|
| Alpha occ. eigenvalues -- | -0.42100 | -0.41942 | -0.41874 | -0.41843 | -0.41717 |
| Alpha occ. eigenvalues -- | -0.41573 | -0.41119 | -0.41091 | -0.40890 | -0.40562 |
| Alpha occ. eigenvalues -- | -0.40344 | -0.40166 | -0.39599 | -0.39257 | -0.39166 |
| Alpha occ. eigenvalues -- | -0.39036 | -0.38929 | -0.38405 | -0.38246 | -0.37708 |
| Alpha occ. eigenvalues -- | -0.37661 | -0.36946 | -0.36693 | -0.36630 | -0.36462 |
| Alpha occ. eigenvalues -- | -0.36339 | -0.36035 | -0.35988 | -0.35209 | -0.35063 |
| Alpha occ. eigenvalues -- | -0.34894 | -0.34627 | -0.34593 | -0.33778 | -0.33761 |
| Alpha occ. eigenvalues -- | -0.33722 | -0.33697 | -0.33165 | -0.33084 | -0.32797 |
| Alpha occ. eigenvalues -- | -0.32786 | -0.32753 | -0.32746 | -0.32195 | -0.32182 |
| Alpha occ. eigenvalues -- | -0.32169 | -0.32157 | -0.31851 | -0.31849 | -0.31827 |
| Alpha occ. eigenvalues -- | -0.31823 | -0.31698 | -0.31697 | -0.31682 | -0.31655 |
| Alpha occ. eigenvalues -- | -0.31646 | -0.31591 | -0.31589 | -0.31567 | -0.31567 |

Alpha  occ. eigenvalues --   -0.30443  -0.30421  -0.29758  -0.29019  -0.28745
Alpha  occ. eigenvalues --   -0.28407  -0.28270  -0.27940  -0.27659  -0.27500
Alpha  occ. eigenvalues --   -0.27365  **-0.25665**
Alpha virt.eigenvalues --   **-0.12366**  -0.05874  -0.04420  -0.03655   0.02140
Alpha virt.eigenvalues --    0.02294   0.08844   0.08848   0.09067   0.09129
Alpha virt.eigenvalues --    0.09153   0.09582   0.09596   0.09882   0.10100
Alpha virt.eigenvalues --    0.10273   0.10603   0.10895   0.10950   0.10978
Alpha virt.eigenvalues --    0.11216   0.11311   0.11547   0.11686   0.11831
Alpha virt.eigenvalues --    0.11891   0.11954   0.12077   0.12565   0.12635
Alpha virt.eigenvalues --    0.12733   0.12791   0.12834   0.12997   0.13627
Alpha virt.eigenvalues --    0.13821   0.14173   0.14289   0.14358   0.14464
Alpha virt.eigenvalues --    0.14629   0.15000   0.15146   0.15616   0.15658
Alpha virt.eigenvalues --    0.15888   0.15941   0.16410   0.16450   0.17018
Alpha virt.eigenvalues --    0.17049   0.17161   0.17452   0.17584   0.17833
Alpha virt.eigenvalues --    0.17880   0.18418   0.18504   0.19058   0.19145
Alpha virt.eigenvalues --    0.19482   0.19534   0.19542   0.19586   0.19687
Alpha virt.eigenvalues --    0.19803   0.19939   0.19958   0.19981   0.19985
Alpha virt.eigenvalues --    0.20026   0.20080   0.20125   0.20193   0.20302

## Calculation of theoretical band gap:

HOMO= - 0.25665*27.2116= - 6.9797754 eV            [27.2116 is the unit conversion constant]
LUMO= - 0.12366*27.2116= - 3.364986546 eV

Band Gap= LUMO-HOMO=$E_g^{Th}$=3.614788944 eV

## Optical Band Gap Calculation from UV-Vis Spectra:

**Liquid State:**

$$\text{Optical Band Gap} = \frac{1240}{\lambda_{onset}} = \frac{1240}{392}$$

$$\mathbf{= 3.16\ eV}$$

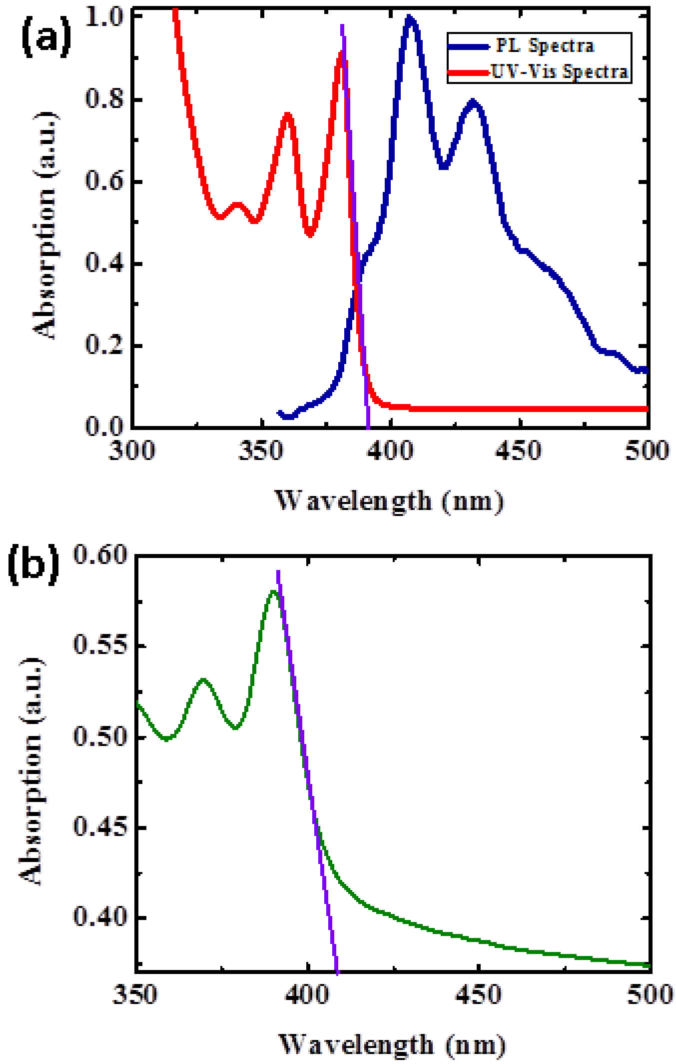



**Figure S3.** (a) Liquid state (b) Solid State UV-Vis spectra of NDI-OD2 molecule.

**Solid State:**

$$\text{Optical Band Gap} = \frac{1240}{\lambda_{onset}} = \frac{1240}{410}$$

$$\mathbf{= 3.02\ eV}$$

## Band Gap Calculation from Electrochemistry:

$E_{LUMO}$=-2.955 eV

$E_{HOMO}$= $E_{LUMO}$-$E_{g\ (opt)}$ [$E_{g\ (opt)}$ **(solid state)** =3.02 eV]

$E_{HOMO}$= (-2.955-3.02) eV = -5.975 eV

## Thermal Deposition Curve of NDI-OD2:

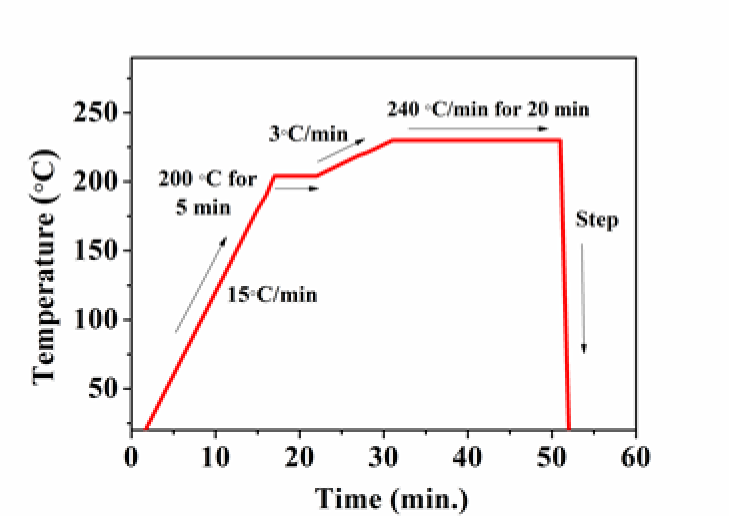



**Figure S4.** Thermal deposition curve of NDI-OD2

## Substrate Cleaning and Film Preparation Technique for Various Spectroscopic and Microscopic Studies:

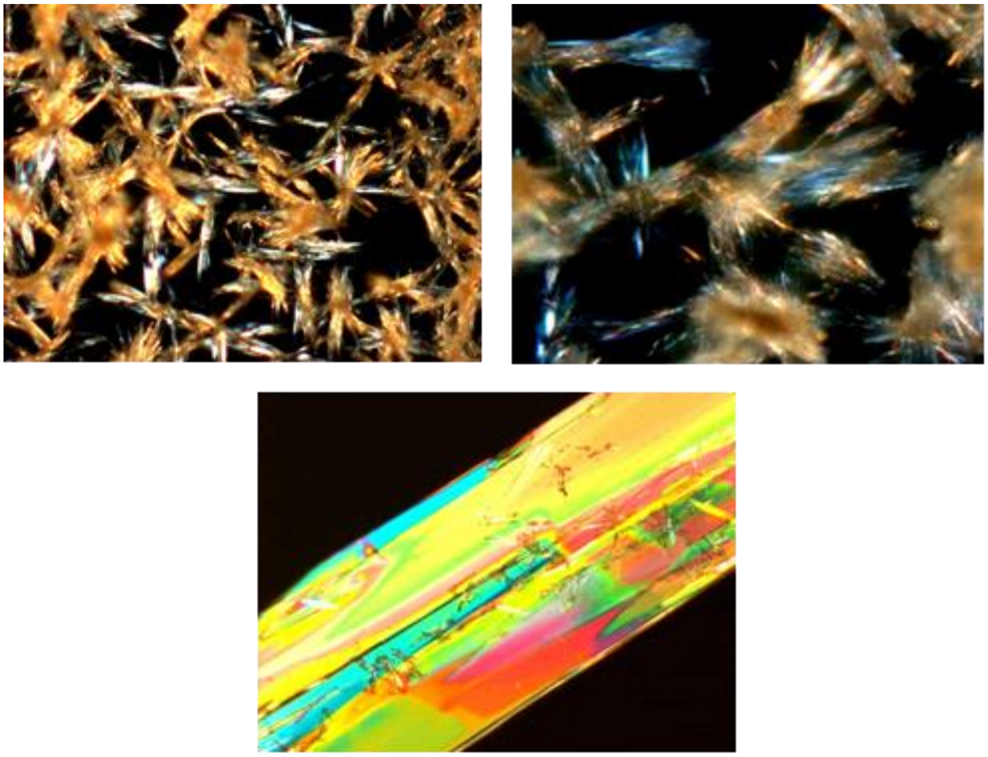
For performing spectroscopic and microscopic studies glass slides were cut into ~1 cm X ~1 cm square substrates. All the substrates were dipped in Piranha solution for approximately 30 min and then cleaned by the following general step wise procedure by sonication in detergent, deionized water, acetone and isopropanol for 20 min each at room temperature. After that the slides are dried in vacuum oven.

**Spin Cast Technique** A solution of NDI-OD2 was prepared in chloroform at a conc. of $10^{-3}$ M. Then the monomer solution was spin-coated on the clean glass slide at 2000 rpm for 2 min by Apex Instrument-SpinNXG-P1 and then dried at room temperature. The thicknesses of the films are found ~60-70 nm when measured by Veeco Dektak 150 Surface Profilometer.

**Thermal Deposition Technique** Thin films of NDI-OD2 monomer were also prepared by thermal deposition technique using Excel Instrument. The monomer was sublimed at 230 °C and the deposition was carried out for 20 min under $10^{-7}$ mbar pressure. The substrate temperature was kept at room temperature. After deposition the thickness of the film (~60 nm ±10) was confirmed by Veeco Dektak 150 Surface Profilometer.

## Polarised Microscopy Images of NDI-OD Monomer:

**(a) Spin cast:**



Single wire of NDI-OD2

**(b) Thermally deposited:**

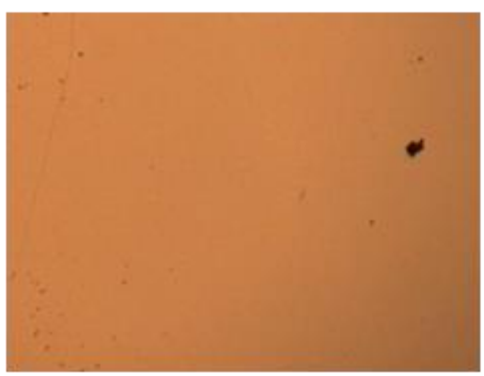
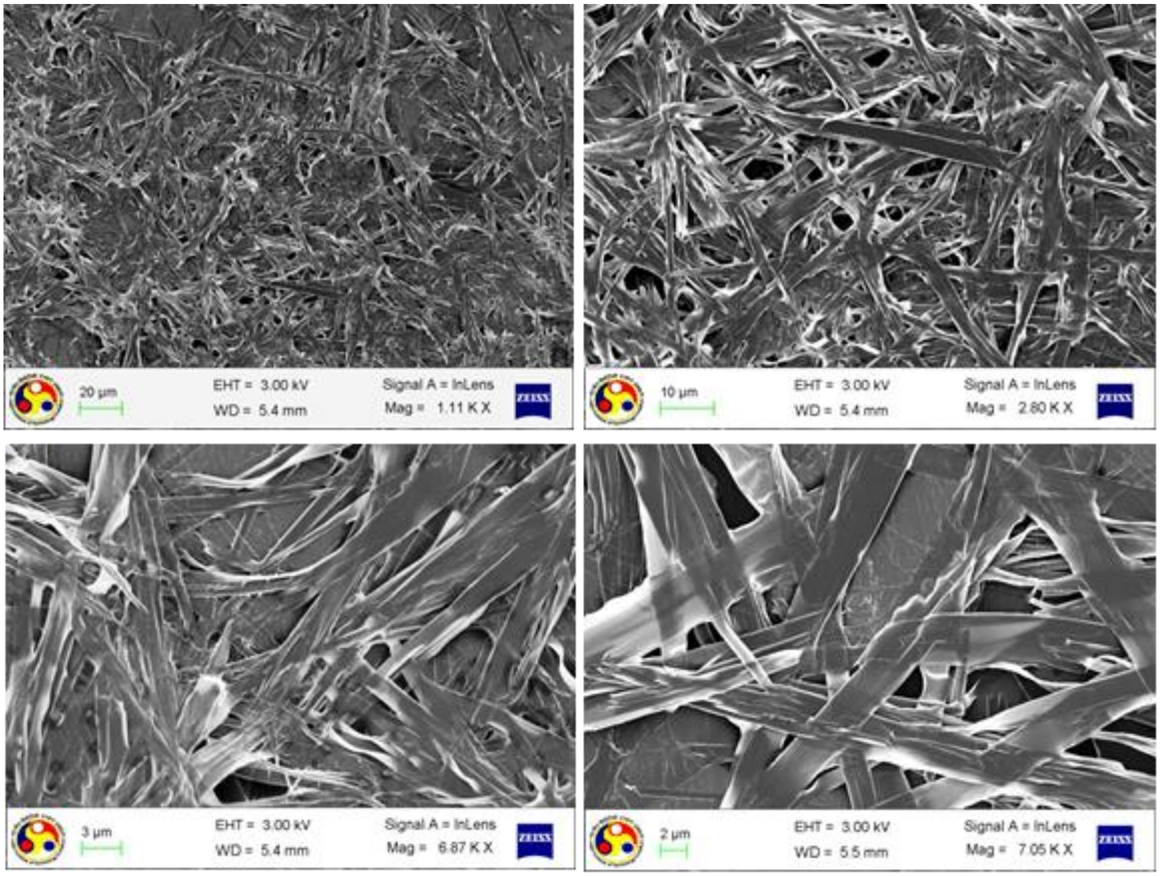


**Figure S5.** Polarized microscopy of (a) spin cast and (b) thermally deposited films of NDI-OD2 monomer in different magnification range.

## FESEM Image of NDI-OD2 Monomer:

### (a) Spin Cast:




### (b) Thermally deposited:

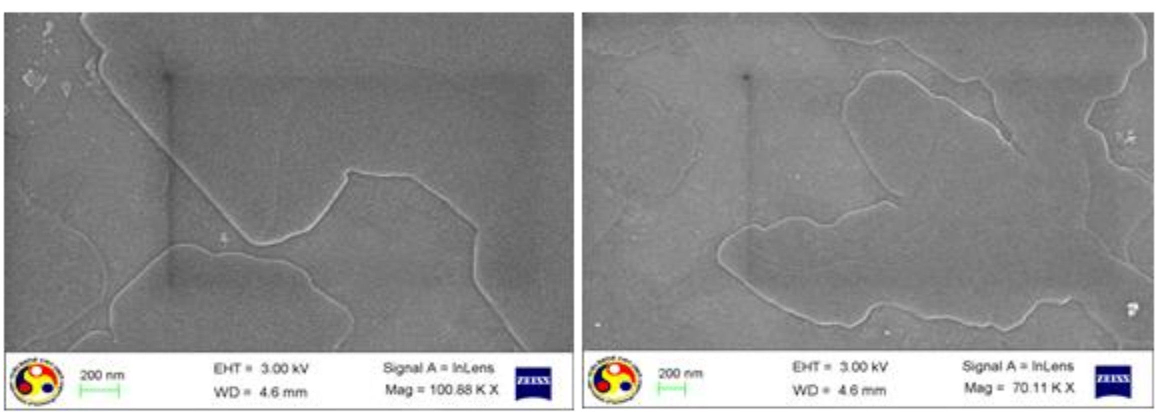



**Figure S6.** FESEM (a) spin cast and (b) thermally deposited films of NDI-OD2 monomer in different magnification range.

**Atomic Force Microscopy Images:**

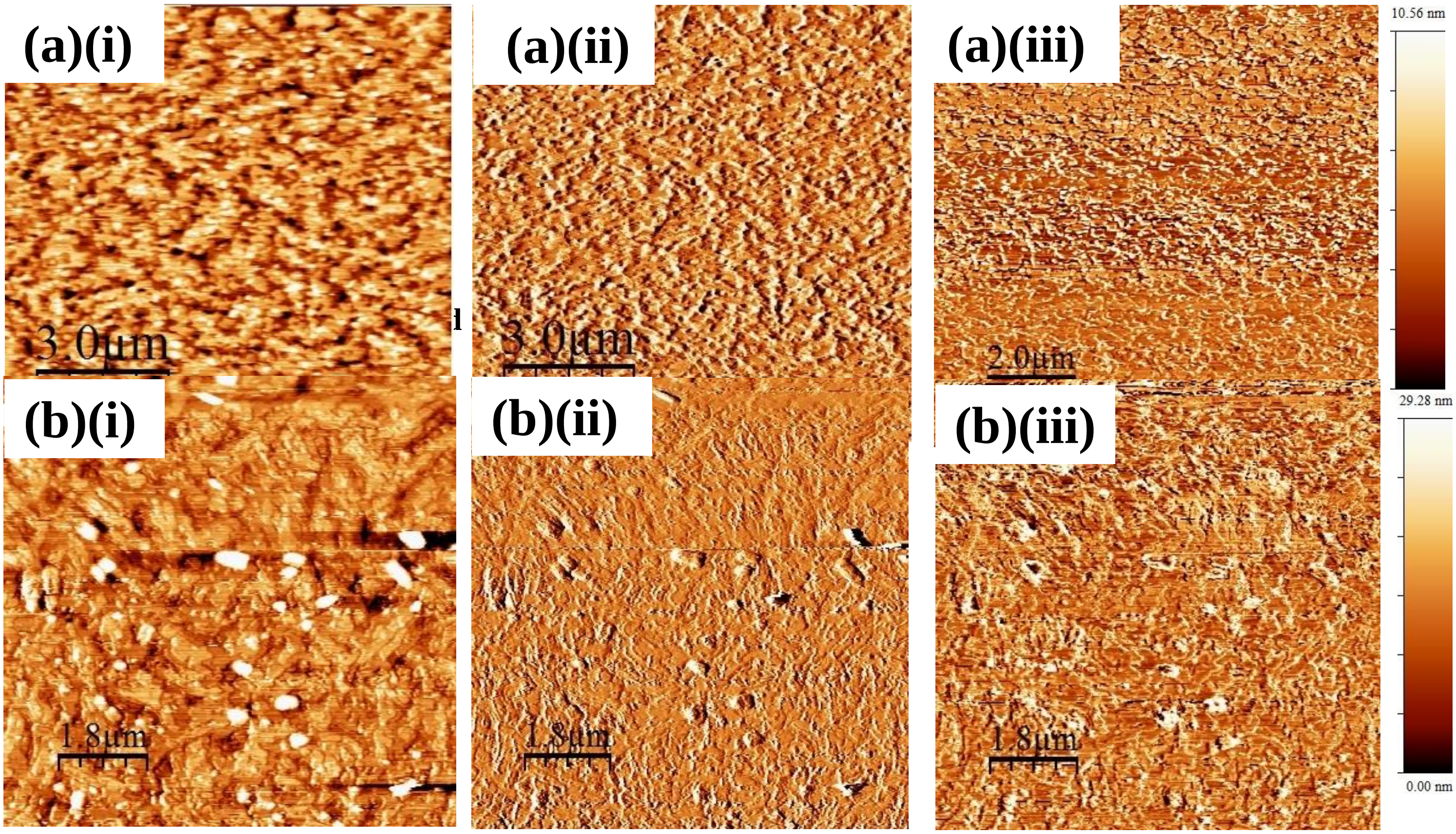



**Figure S7**. AFM (a) (i) topography, (ii) amplitude, (iii) phase images of spin cast and (b) (i) topography, (ii) amplitude, (iii) phase images of thermally deposited films of NDI-OD2 monomers respectively.

## Transmission Electron Microscopy Images:

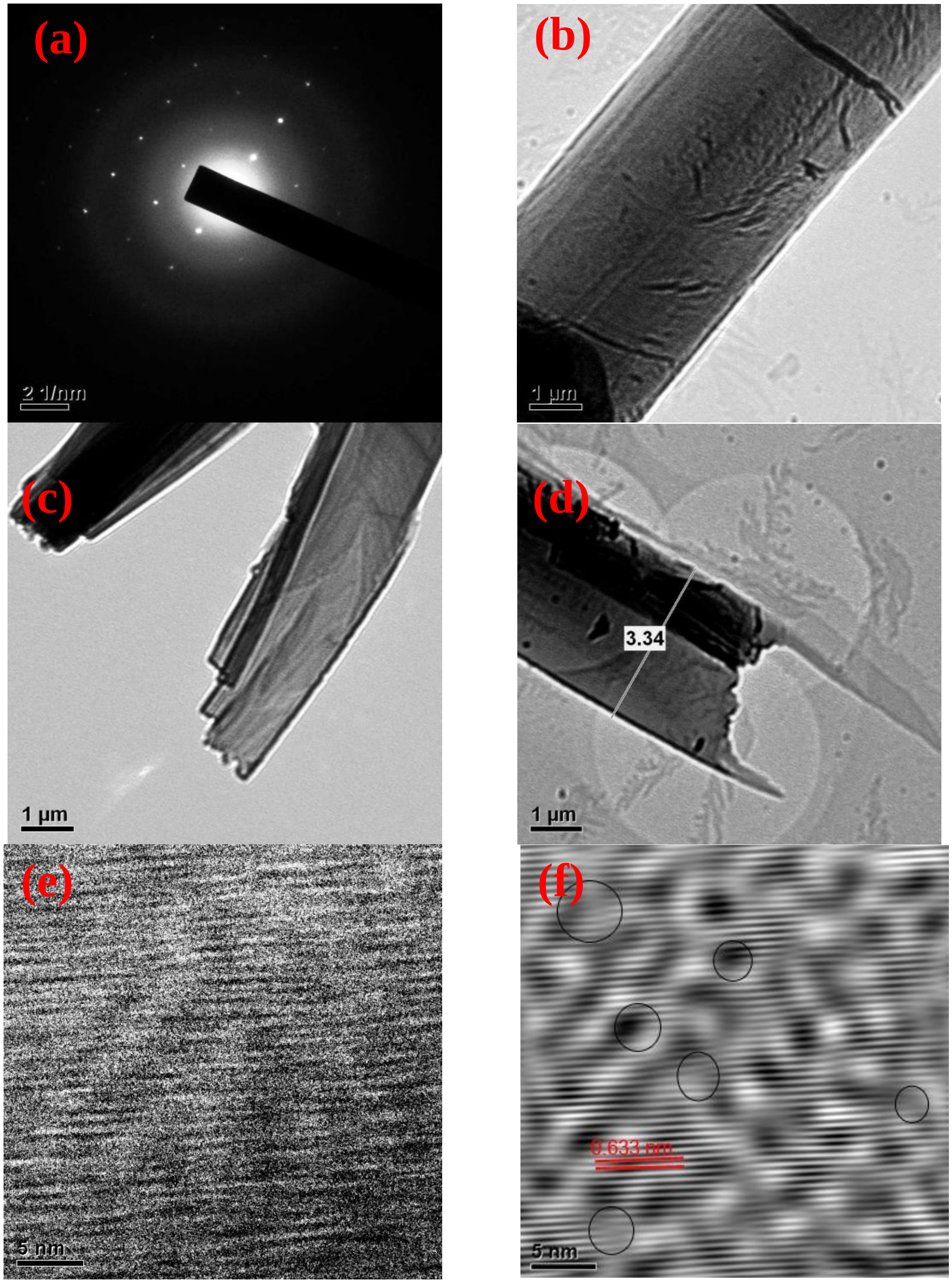
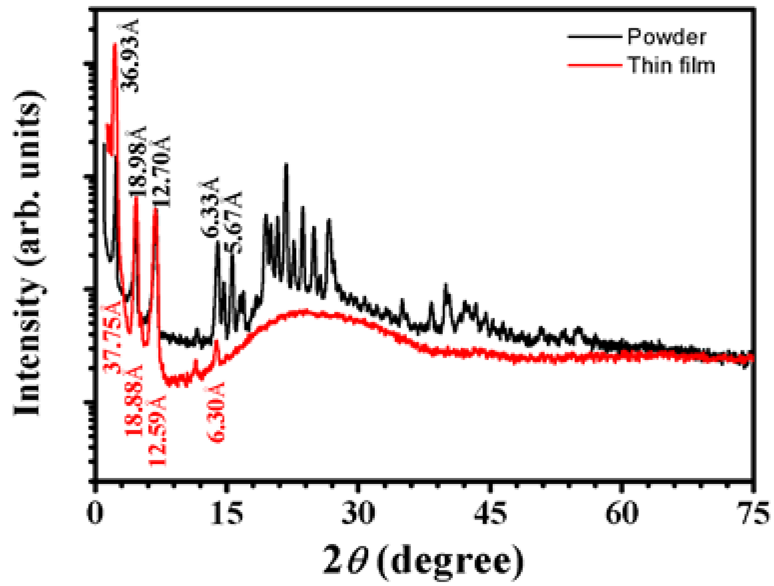



**Figure S8**. TEM (a) SAED pattern (b), (c), (d) TEM images at different portion of the film (e), (f) HRTEM images of NDI-OD2.

**XRD Data:**

(a)




(b)

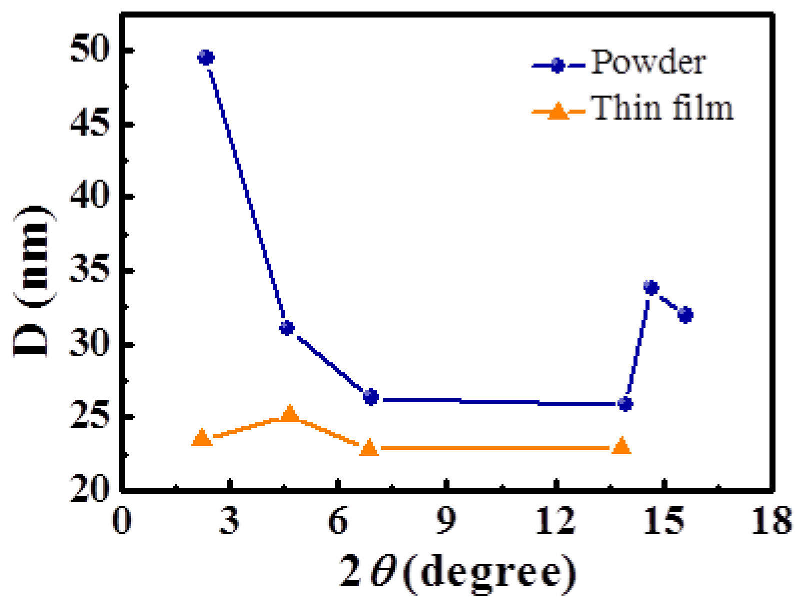



**Figure S9**. (a) XRD pattern (b) Particle size vs. 2$\theta$ graph of NDI-OD2.

## Device Fabrication:

### Procedure:

Glass slides were cut into ~1 cm X ~2 cm rectangle dimensions. Similar to the procedure followed for cleaning the glass substrates for microscopic and spectroscopic studies, the same general substrate cleaning method was applied here followed by drying in vacuum oven for 20 min. Glass substrates of dimensions ~1 cm X ~2 cm were cut and cleaned using the following procedure. The substrates were sonicated for 10 minutes in detergent, followed by step wise sonication with deionized water, acetone and isopropanol for 20 minutes each at room temperature followed by drying in a vacuum oven for 20 minutes. An L-shaped aluminum gate electrode film (100 nm) was thermally deposited on the substrate under $10^{-6}$ mbar pressure. A spin coated film of polyvinyl alcohol (PVA) with thickness of (~1 µm, 1000 rpm) was deposited as a dielectric material having capacitance ~8.854 nF/cm$^2$. Thin film of NDI-OD2 (~60 nm ±10 nm) was thermally deposited ($10^{-7}$ mbar ) on the dielectric layer followed by aluminum source and drain contacts (100 nm) deposition on this NDI-OD2 organic layer through a shadow mask with channel length (L) and width (W) of 50 µm and 1 mm respectively. Electrical measurements of OTFT devices were carried out under vacuum (~$10^{-4}$ mbar) using a Keithley 4200-SCS semiconductor parameter analyzer. The field-effect mobility was calculated in the saturation regime by using the equation $I_{DS} = (\mu_e W C_i/2L)(V_G - V_T)^2$, where $I_{DS}$ is the drain-source current, $\mu_e$ is the field-effect mobility, $W$ is the channel width, $L$ is the channel length, $C_i$ is the capacitance per unit area of the gate dielectric layer, $V_G$ is the gate voltage, and $V_T$ is the threshold voltage. For analyzing the moisture related stability of the fabricated OTFT devices, the tests were performed at an interval of 24 hours with the devices being continuously exposed to environment having >80% humidity levels at room temperature until the devices degraded completely.

## Device Block Diagram

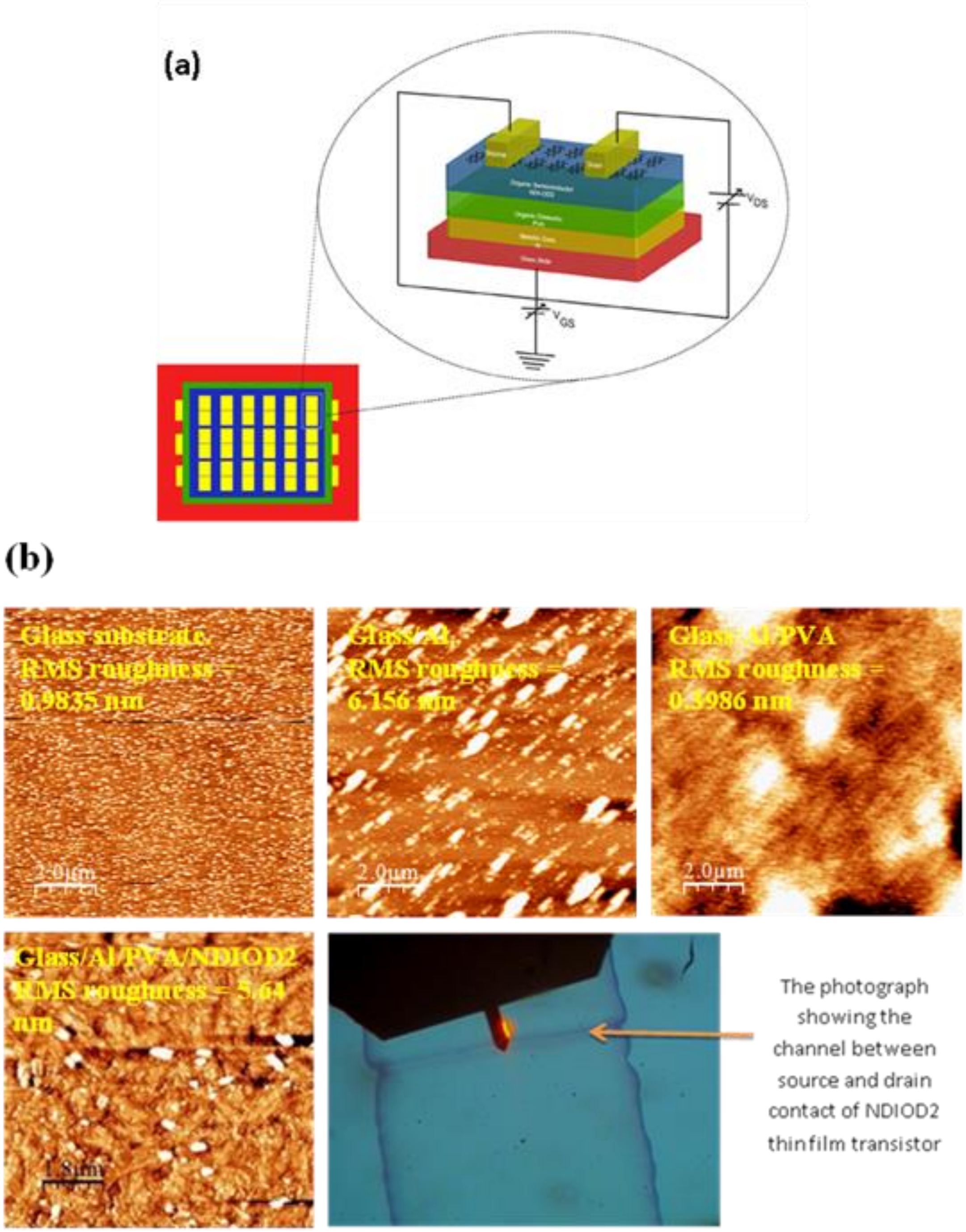
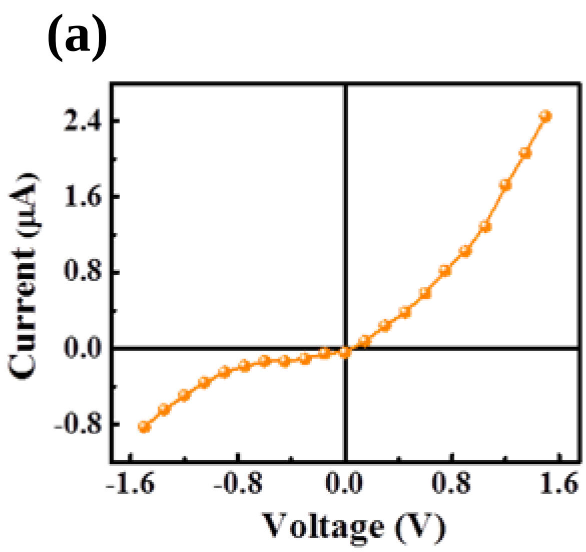
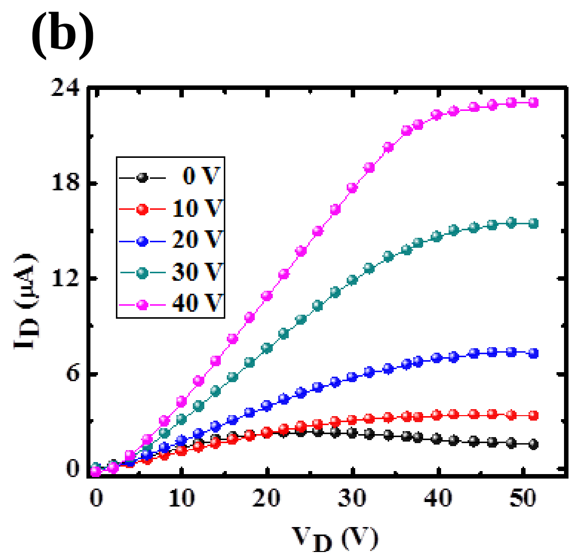



**Figure S10**. (a) Schematic of the device and (b) Layer-by layer AFM images of the of the NDI-OD2 monomer based OTFT device.

**I-V Characteristics** **Output Characteristics**




**Transfer Characteristics**

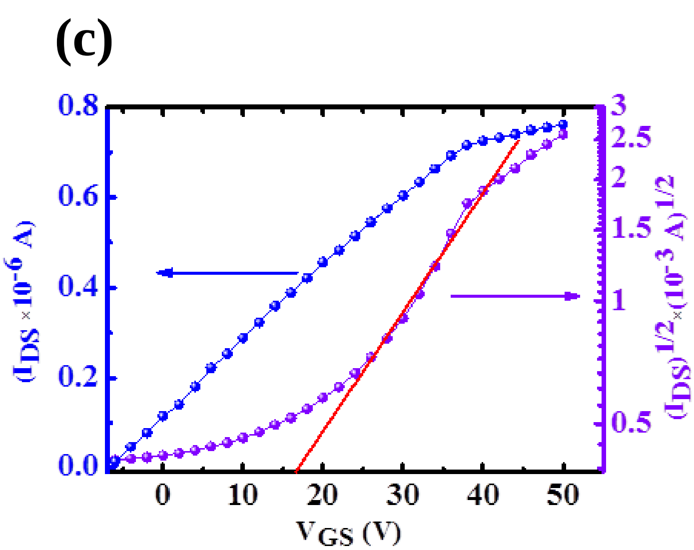



**Figure S11**. (a) I-V Characteristic (b) Output characteristics and (c) Transfer characteristics of the NDI-OD2 monomer respectively.

**Degradation Data:**

**Transfer Characteristics:**

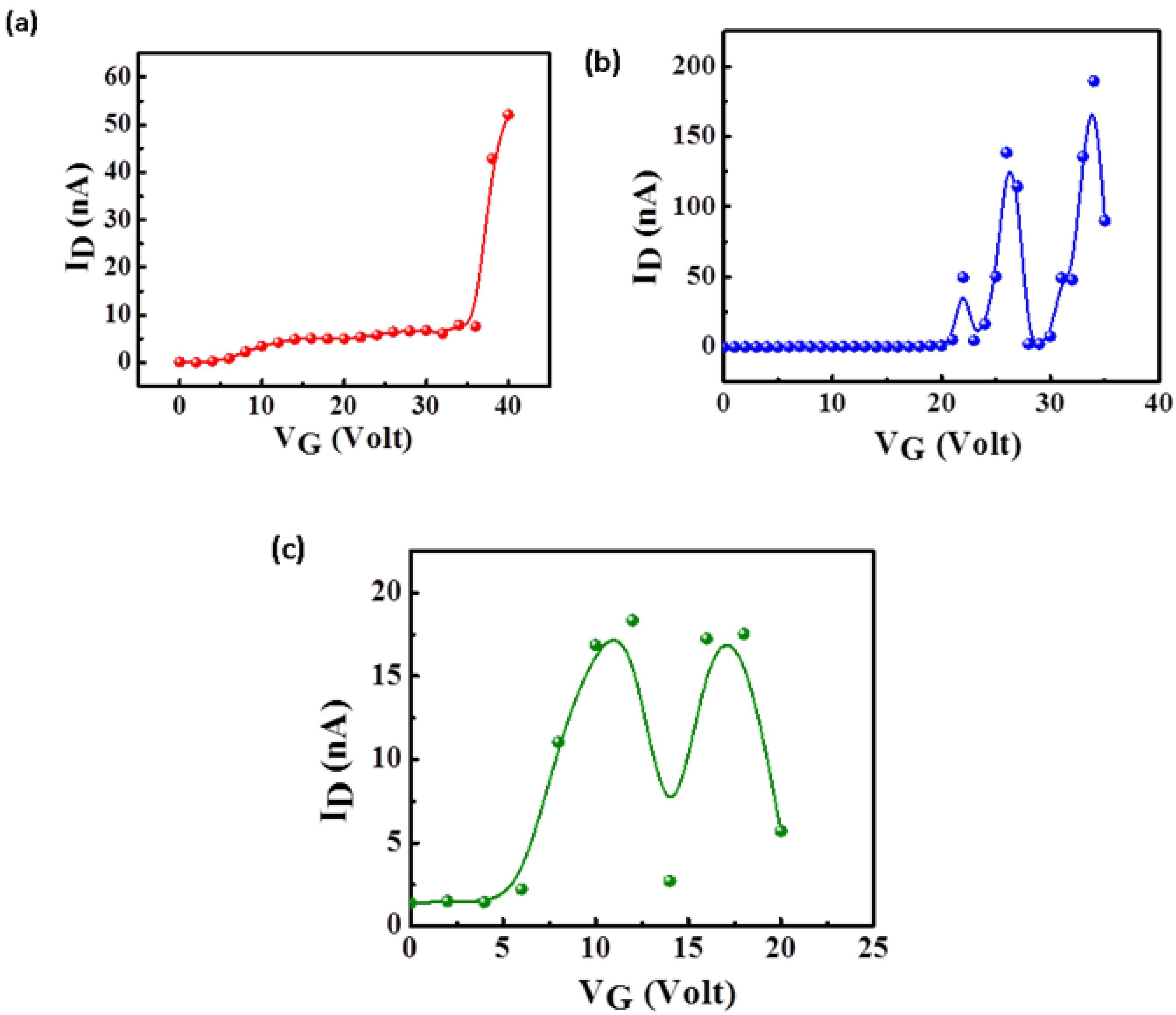



**Figure S12**. Transfer Characteristics of the NDI-OD2 OTFT device (a) after 4 days (b) after 7 days and (c) after 10 days exposure to moisture.