

Supporting Information

Isoindigo-Based Semiconducting Polymers using Carbosilane Side Chains for High Performance Stretchable Field-Effect Transistors

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Monomer synthesis

Synthesis of dihexyl(methyl)silane (1a)

A mixture of dichloromethylsilane (3.99 g, 34.7 mmol) and hexylmagnesium bromide (13.1 g, 69.4 mmol) in tetrahydrofuran (85 mL) was prepared in a two-neck flask at 0 °C. The mixture was warmed up to room temperature and reacted for additional 2 h. Then the mixture was quenched using methanol and the solvent (i.e. tetrahydrofuran and methanol) was evaporated under vacuum. Next, the mixture was extracted with water and diethyl ether, and the organic extract was dried over MgSO_4 to remove water, and the solvent was evaporated under vacuum. The crude products were purified by distillation to obtain 1a (6.62 g, 89 %) as a colorless oil. $^1\text{H-NMR}$ (400 MHz, CDCl_3), δ (ppm): 3.75 (m, 1H), 1.38-1.21 (m, 16H), 0.94-0.83 (m, 6H), 0.64-0.50 (d, 4H), 0.09-0.00 (m, 3H).

Synthesis of dioctyl(methyl)silane (1b)

A mixture of dichloromethylsilane (3.71 g, 32.3 mmol) and octylmagnesium bromide (14.1 g, 64.6 mmol) in tetrahydrofuran (85 mL) was prepared in a two-neck flask at 0 °C. The mixture was warmed up to room temperature and reacted for additional 2 h. Then the mixture was quenched using methanol and the solvent (i.e. tetrahydrofuran and methanol) was evaporated under vacuum. Next, the mixture was extracted with water and diethyl ether, and the organic extract was dried over MgSO_4 to remove water, and the solvent was evaporated under vacuum. The crude products were purified by distillation to obtain 1b (6.90 g, 79 %) as a colorless oil. $^1\text{H-NMR}$ (400

MHz, CDCl₃), δ (ppm): 3.75 (m, 1H), 1.41-1.20 (m, 24H), 0.99-0.82 (m, 6H), 0.64-0.48 (d, 4H), 0.14-0.00 (m, 3H).

Synthesis of (6-bromohexyl)dihexyl(methyl)silane (2a)

A mixture of 1a (2.18 g, 10.2 mmol) and 6-bromo-1-hexene (2.49 g, 15.3 mmol) was firstly prepared in a two-neck flask and purged nitrogen for 5~10 min. 26 mL toluene and 3~4 drops of Karstedt's catalyst were added subsequently, and the mixtures was heated up to 50 °C and reacted overnight. Afterward, the crude products were purified by chromatography using hexane as eluent to obtain 2a (3.30 g, 86 %) as a transparent oil. ¹H-NMR (400 MHz, CDCl₃), δ (ppm): 3.40 (m, 2H), 1.92-1.81 (m, 2H), 1.49-1.18 (m, 22H), 0.92-0.83 (m, 6H), 0.52-0.40 (d, 6H), -0.10 (d, 3H).

Synthesis of (6-bromooctyl)dioctyl(methyl)silane (2b)

A mixture of 1b (3.12 g, 11.5 mmol) and 8-bromo-1-octene (3.30 g, 17.3 mmol) was firstly prepared in a two-neck flask and purged nitrogen for 5~10 min. 26 mL toluene and 3~4 drops of Karstedt's catalyst were added subsequently, and the mixtures was heated up to 50 °C and reacted overnight. Afterward, the crude products were purified by chromatography using hexane as eluent to obtain 2b (3.60 g, 68 %) as a transparent oil. ¹H-NMR (400 MHz, CDCl₃), δ (ppm): 3.40 (m, 2H), 1.90-1.81 (m, 2H), 1.45-1.19 (m, 34H), 0.90-0.78 (m, 6H), 0.50-0.41 (d, 6H), -0.12 (d, 3H).

Synthesis of IID-C6

A suspension of 6,6'-dibromoisindigo (1.46 g, 3.5 mmol) and potassium carbonate (1.9 g, 14 mmol) was prepared in 60 mL dimethylformaldehyde, then 2a (3.15 g, 8.3 mmol) was added through a septum under an nitrogen atmosphere at room temperature. The mixture was heated up and stirred for 12 h at 100 °C and then poured into methanol (200 mL). The precipitates were collected by vacuum filtration and extracted using methylene chloride and water. The crude products were further purified by chromatography using methylene chloride and hexane (v:v = 1:2) as eluent to obtain IID-C6 (1.90 g, 54 %) as a red powder. ¹H-NMR (400 MHz, CD₂Cl₂), δ (ppm): 9.08 (d, 2H), 7.15, (dd, 2H), 6.98 (d, 2H), 3.70 (d, 4H), 1.75-1.15 (m, 48H), 1.00-0.78 (m, 12H), 0.60-0.35 (m, 12H), -0.10 (d, 6H).

Synthesis of IID-C8

A suspension of 6,6'-dibromoisindigo (0.85 g, 2.0 mmol) and potassium carbonate (1.1 g, 8.0 mmol) was prepared in 45 mL dimethylformaldehyde, then 2b (2.22 g, 8.3 mmol) was added through a septum under an nitrogen atmosphere at room temperature. The mixture was heated up and stirred for 12 h at 100 °C and then poured into methanol (150 mL). The precipitates were collected by vacuum filtration and extracted using methylene chloride and water. The crude products were further purified by chromatography using methylene chloride and hexane (v:v = 1:2) as eluent to obtain IID-C8 (1.50 g, 63 %) as a red powder. ¹H-NMR (400 MHz, CDCl₃), δ (ppm):

9.08 (d, 2H), 7.15, (dd, 2H), 6.98 (d, 2H), 3.70 (d, 4H), 1.72-1.60 (m, 4H), 1.40-1.15 (m, 66H),
0.85-0.78 (m, 14H), 0.48-0.35 (m, 12H), -0.12 (d, 6H).

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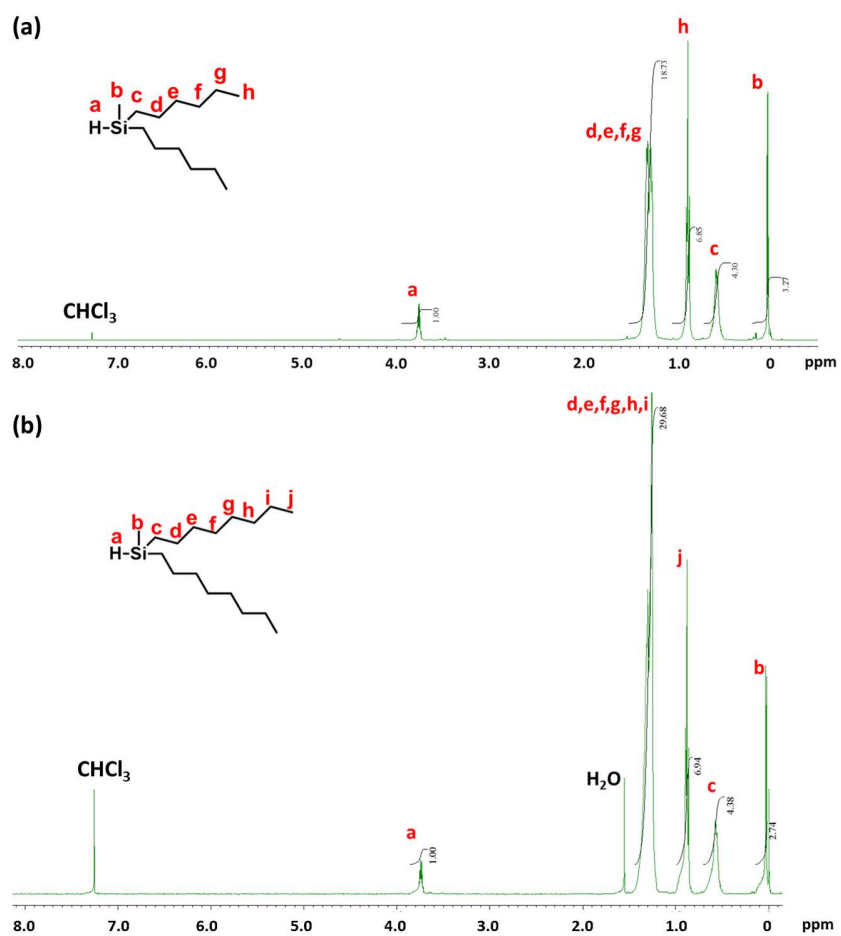


Figure S1. ^1H -NMR spectra of compounds (a) 1a and (b) 1b in CDCl_3 , respectively.

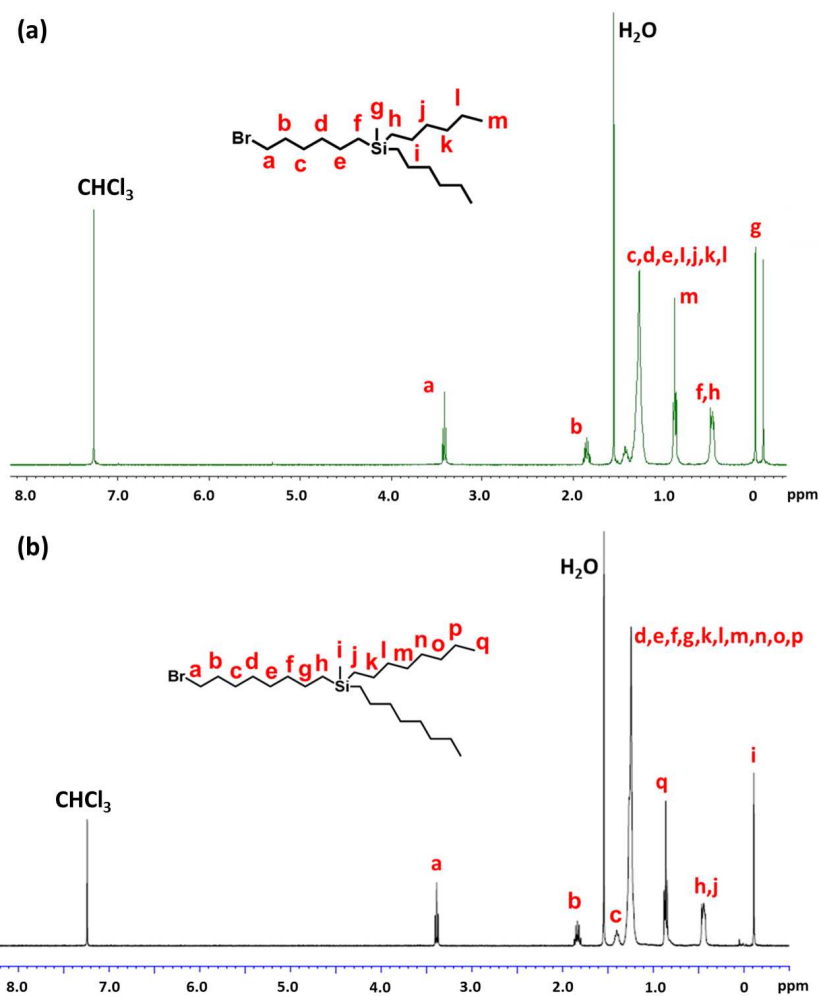


Figure S2. ^1H -NMR spectra of compounds (a) 2a and (b) 2b in CDCl_3 , respectively.

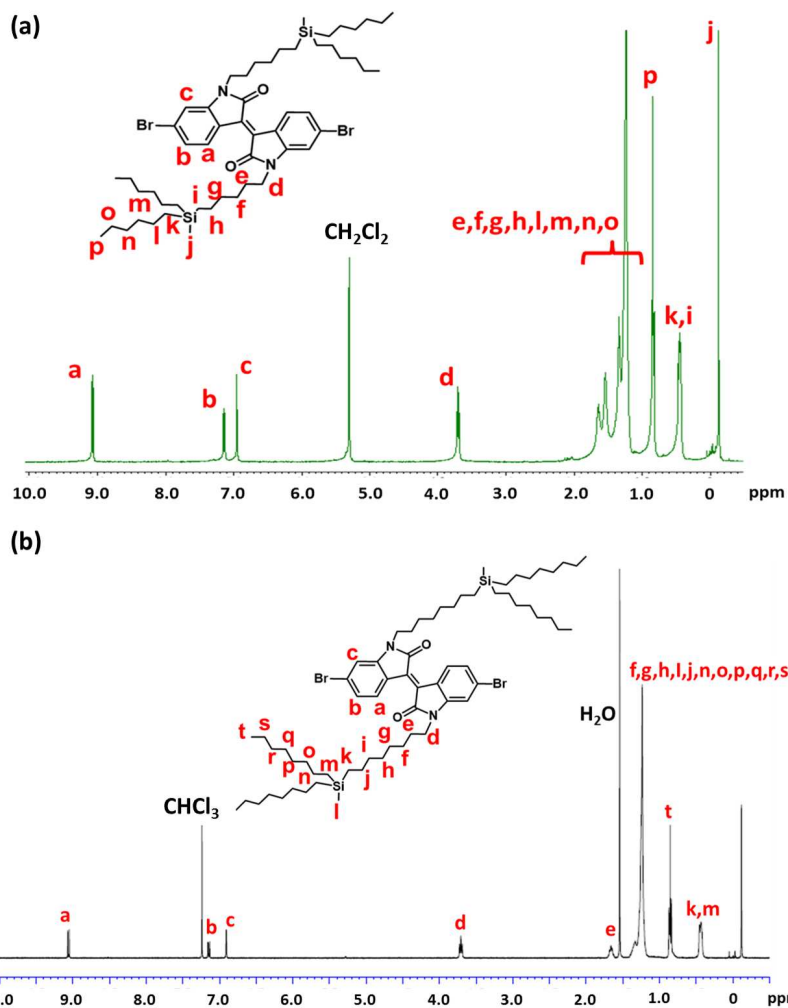


Figure S3. ^1H -NMR spectra of compounds (a) IID-C6 in CD_2Cl_2 and (b) IID-C8 in CDCl_3 , respectively.

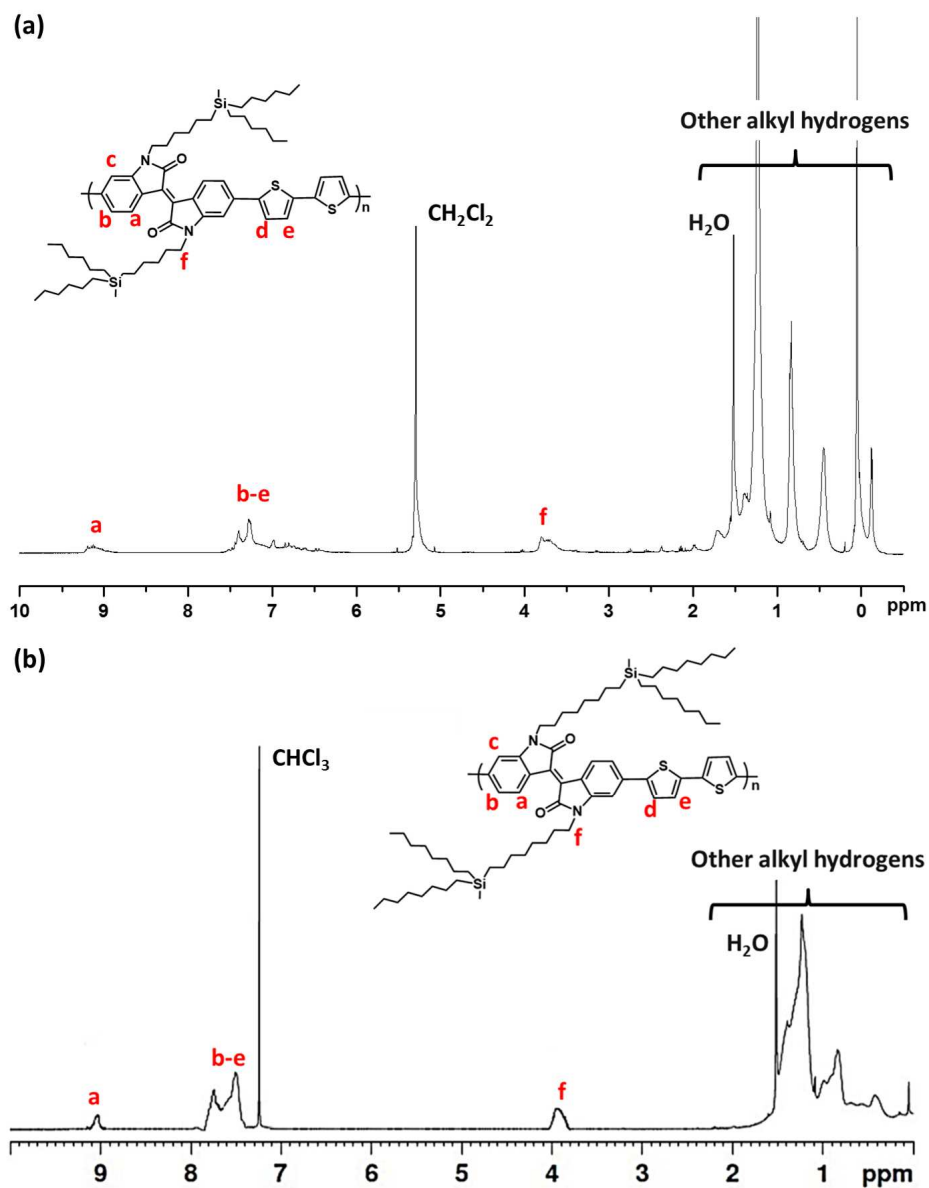


Figure S4. ^1H -NMR spectra of (a) PII2T-C6 in CD_2Cl_2 and (b) PII2T-C8 in CDCl_3 , respectively.

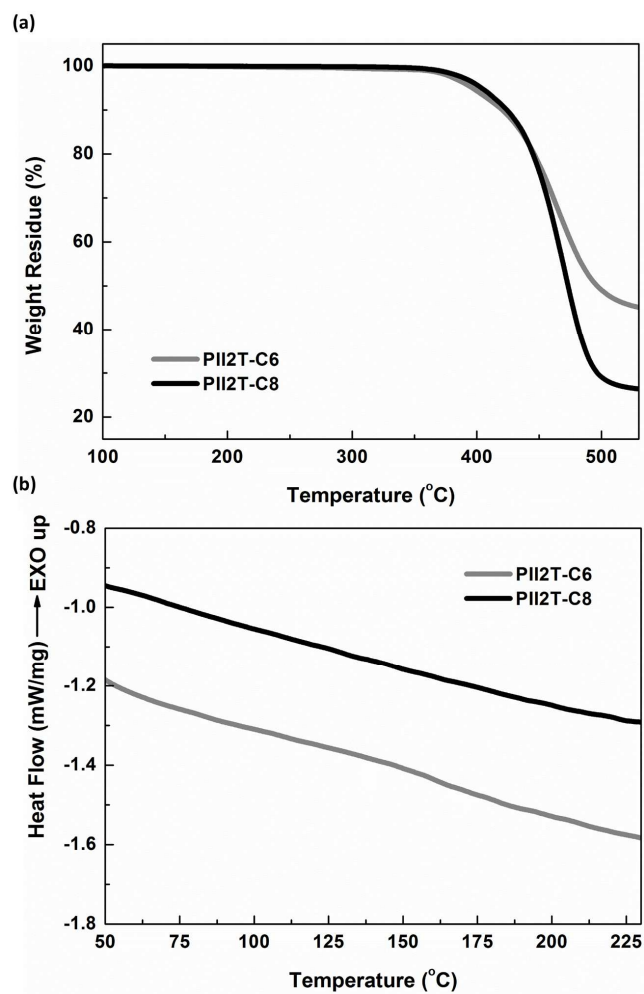


Figure S5. (a) TGA curves and (b) DSC traces of PII2T-C6 and PII2T-C8.

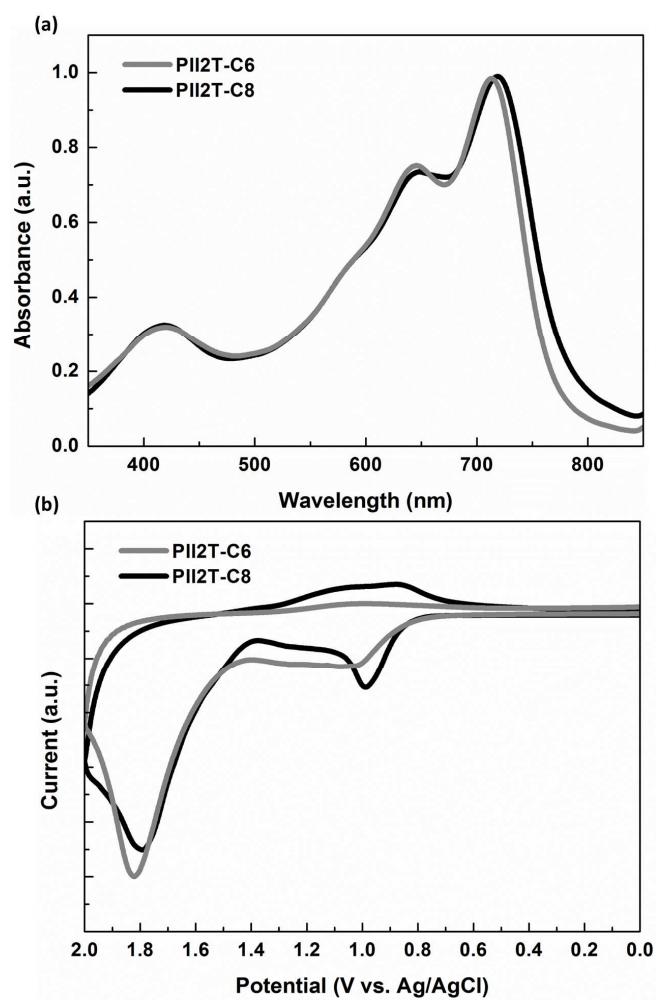


Figure S6. (a) Solid state UV-Vis absorption spectra and (b) CV curves of PII2T-C6 and PII2T-C8.

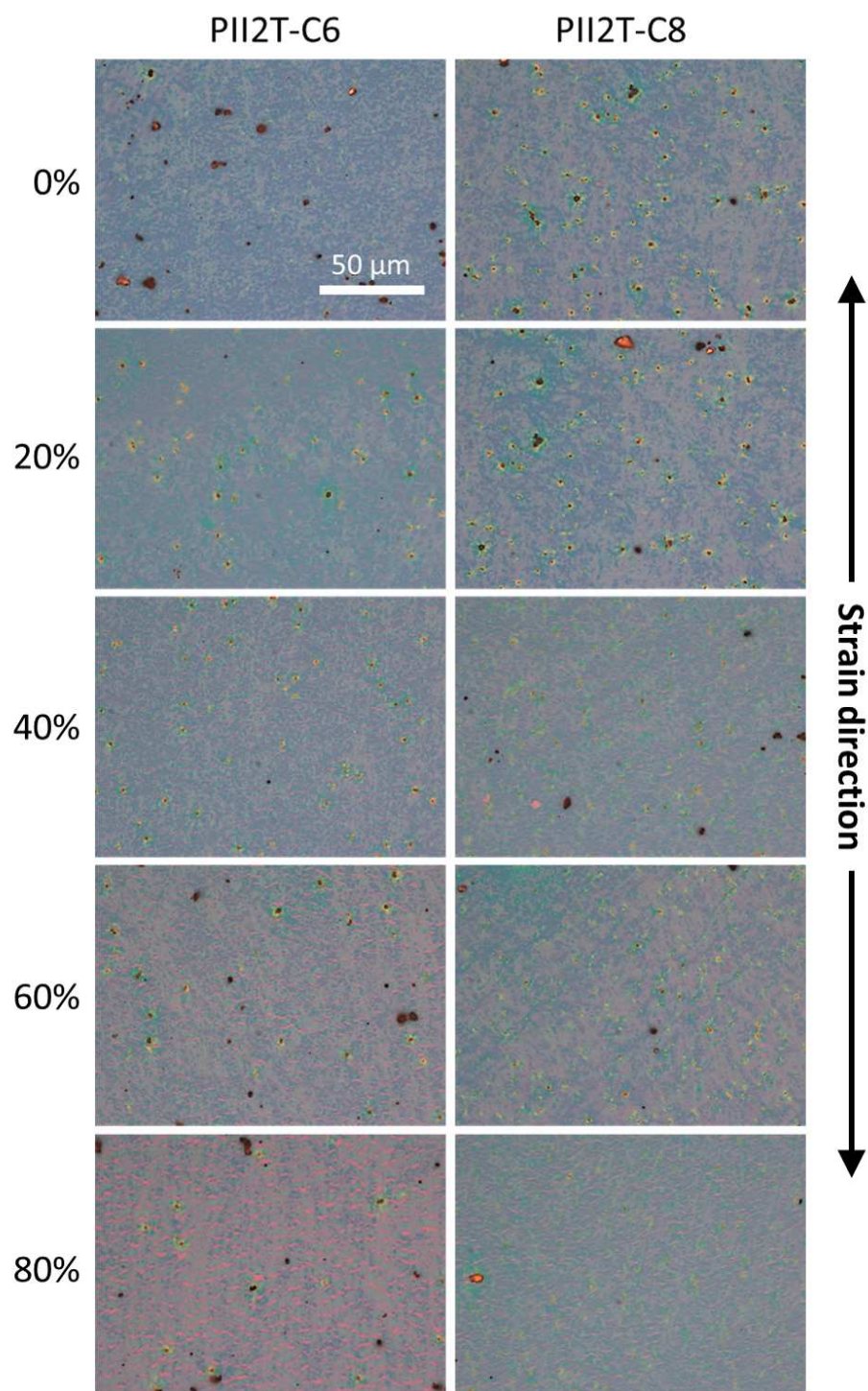


Figure S7. Optical microscopy images of PII2T-C6 and PII2T-C8 thin films under different strain levels.

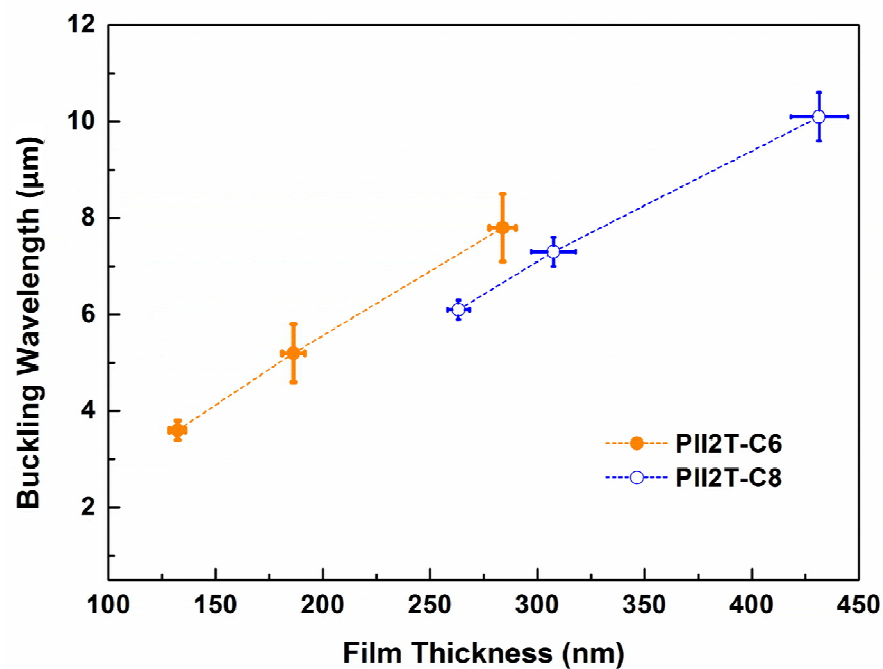


Figure S8. Mechanical properties of PII2T-C6 and PII2T-C8 thin films. The relationship between buckling wavelength and film thickness, which can calculate the tensile modulus using reported method (*Adv. Funct. Mater.*, 2014, **24**, 1169). Note that the Poisons ratio of PDMS and conjugated polymer is assumed as 0.5 and 0.35, respectively, and the elastic modulus of PDMS is measured to be 1.4 MPa.

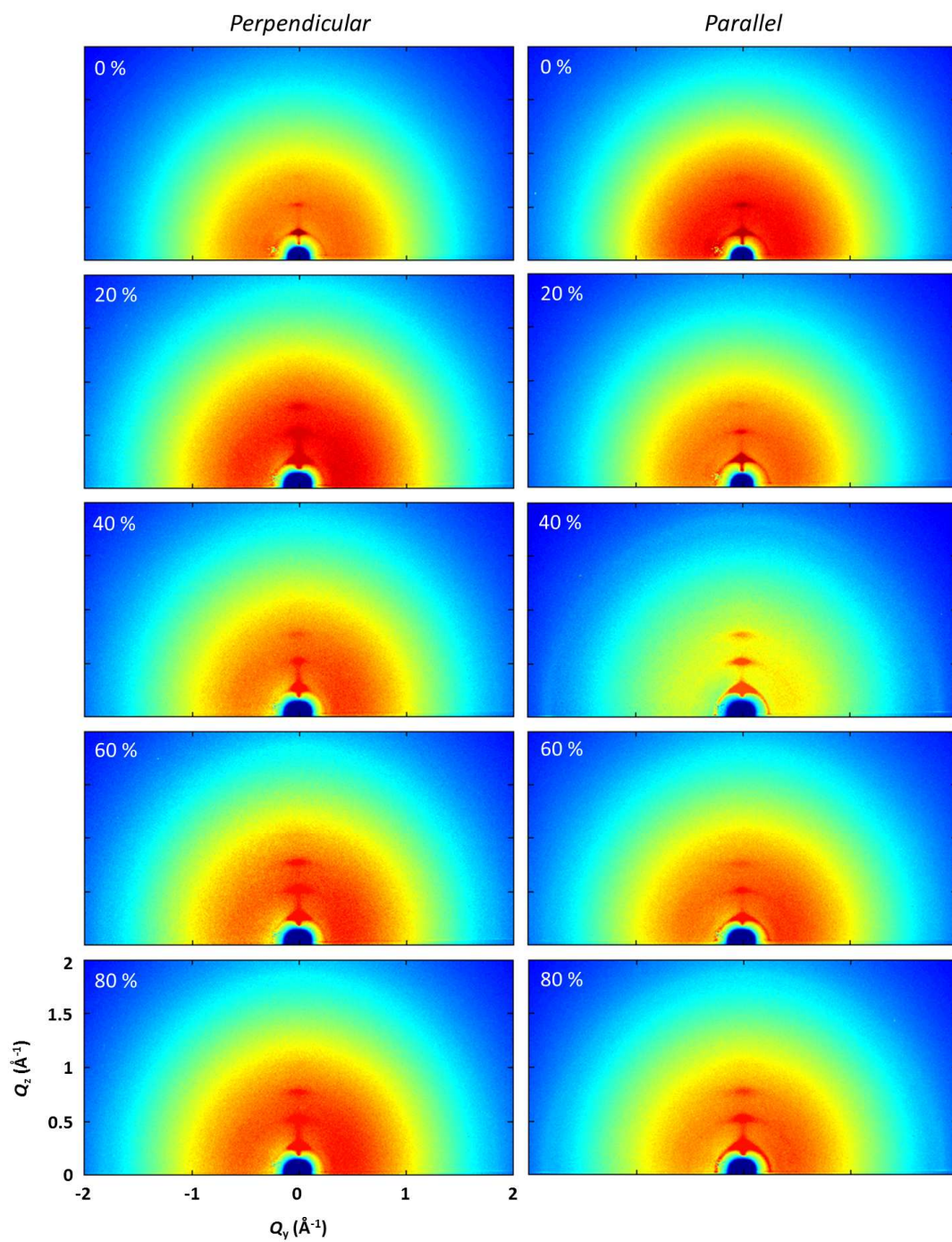


Figure S9. 2D GIXD patterns of PII2T-C6 thin films under different strain levels as the X-ray incidence light perpendicular or parallel to the thin film stretching direction.

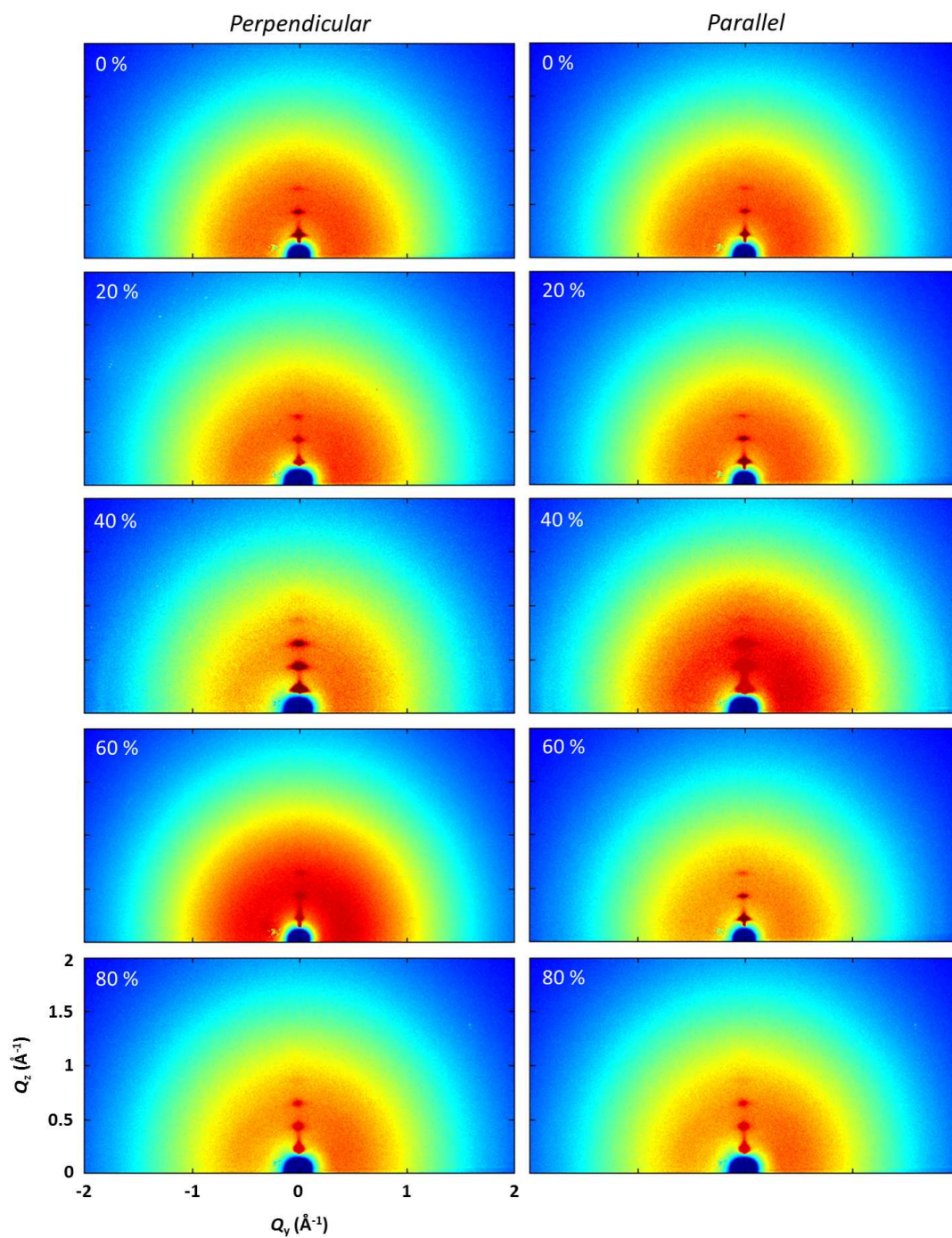


Figure S10. 2D GIXD patterns of PII2T-C8 thin films under different strain levels as the X-ray incidence light perpendicular or parallel to the thin film stretching direction.

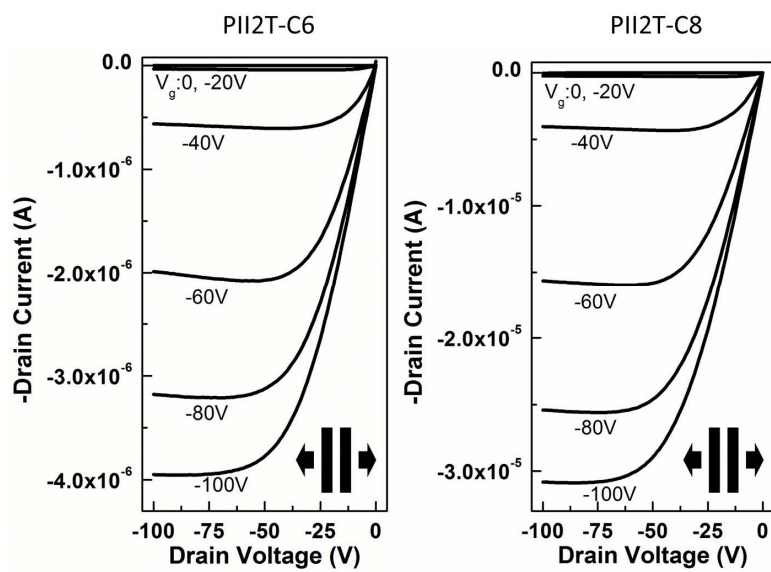


Figure S11. Output characteristics of the FET devices based on PII2T-C6 and PII2T-C8 thin films with 100% strain.