Supporting information for

Synthesis and Properties of Isoindigo and Benzo[1,2-b:4,5b']bis[b]benzothiophene oligomers

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1. Materials and Methods

All chemicals were purchased from commercial suppliers and used as received unless otherwise specified. Column chromatography was carried out with silica gel for flash chromatography from VWR Scientific. ¹H and ¹³C NMR spectra were recorded on a Bruker Model 400 spectrometer and high temperature ¹H NMR was recorded on a Bruker Model 500 spectrometer. UV-vis absorption spectra were recorded on a UV-1601 Shimadzu UV-vis spectrometer. The melting point of compounds have been obtained using SGW X4 Micro Melting Point Apparatus. Cyclic voltammetry (CV) was performed using an Autolab PGSTAT101 potentiostat with a standard three-electrode system consisting of a cylindrical platinum working electrode, platinum mesh counter electrode and Ag/Ag+ reference electrode, calibrated against ferrocene. Measurements were carried out on the acceptors $(3 \times 10^{-4} \text{ M})$ in deoxygenated dichloromethane with 0.3 М of tetrabutylammonium anhydrous and hexafluorophosphate (TBAPF₆) as the supporting electrolyte. HOMO and LUMO energy levels were calculated from the equations: $E_{LUMO} = -(E_{red} - E_{Fc} + 4.8)$ eV and $E_{HOMO} = -(E_{ox} - E_{Fc} + 4.8)$ eV, where E_{red} and E_{ox} are taken from the onset of reduction and oxidation, respectively, and E_{Fc} is the half-wave potential of ferrocene.

Films of the semiconductors were spin-coated from toluene solution (10 mg/mL, 3000 r/min, 40-60 nm) onto Si/SiO₂ (300 nm) substrates modified with octadecyltrichlorosilane (OTS). Source/drain electrodes with optimal width/length (W/L) of 1400 μ m/50 μ m for Compound **6**, electrodes were sputtered and patterned by a lift-off technique. All devices were measured in insert atmosphere with Bottom-Gate Bottom-Contact configuration. Prior to the deposition of polymer thin films, the OTS modified Si/SiO₂ substrate was cleaned with hexane, chloroform, and ethanol. Then, thin films were produced on Si/SiO₂ substrates through spin-coating. Electrical characteristics of the devices were recorded with a Keithley 4200-SCS semiconductor parameter analyser and a Micromanipulator 6150 probe station in a glove box at room temperature.

2. Partial ¹H NMR spectra of the compounds



Figure S1. Partial ¹H NMR spectra of 8, 9 in 1,1,2,2-tetrachloroethane- d_2 at room temperature and 10 in 1,1,2,2-tetrachloroethane- d_2 at 403 K.

3. DFT Calculations

All geometries were fully optimized at the tuned ω B97XD/6-31G(d,p) level of theory. The long alkyl side-chains were replaced by methyl groups to reduce computational costs. The range-separation parameter (ω) was optimized in the presence of a dielectric medium using the polarizable continuum model (PCM) for each molecule using the IP-tuning method.^[1,2] Chloroform is used as implicit solvent in all DFT/PCM calculations. The optimal ω values for 6, 8, 9, and 10 are 0.011, 0.008, 0.007, and 0.004 bohr⁻¹, respectively. All calculations were performed with the Gaussian09 software.^[3]



10 (r= 1.9 Å, d= 10°)

Figure S2: Optimized geometric structures for the compounds 6, 8, 9 and 10 as determined at ω B97XD/6-31G(d,p) level of theory.



Figure S3: Simulated absorption spectra for the **6**, **8**, **9**, and **10**, as calculated at the TD-OT- ω B97XD/6-31G(d,p) in chloroform solvent. The spectra are simulated based on a Gaussian-function convolution (FWHM=0.3 eV) of the molecules vertical excitation energies and oscillator strengths.







8 (S₀->S₁) (2.16 eV 570 nm) (f=0.11)



9 (S₀->S₁) (2.08 eV 595 nm) (f=0.21)





Figure S4: Illustration of the hole and electron wavefunctions (isovalues 0.02 a.u.) determined at the TD-OT- ω B97XD/6-31G(d,p) level of theory for the lowest optical transitions in 6, 8, 9, and 10. The contributions of the various hole-electron configurations are given in percentages.



6 (S₀->S₆) (3.05 eV 400 nm) (f=0.41)



8 (S₀->S₄) (2.74 eV 450 nm) (f=0.73)



9 (S₀->S₆) (2.62 eV 470 nm) (f=0.68)



10 (S₀->S₅) (2.31 eV 535 nm) (f=2.22)

Figure S5: Illustration of the hole and electron wavefunctions (isovalues 0.02 a.u.) determined at the TD-OT- ω B97XD/6-31G(d,p) level of theory for various S₀-> S_n optical transitions in 6, 8, 9, and 10. The contributions of the various hole-electron configurations are given in percentages.



Figure S6. Illustration of the HOMO and LUMO wavefunctions together with their energies (in eV) as Pictorial representation of single-electron HOMO and LUMO wavefunction distribution and their energy levels determined at the OT(chloroform)- ω B97XD/6-31G(d,p) level of theory. Long The long alkyl side-chains were substituted with methyl groups.

4. Absorption spectra of thin films of the compounds



Figure S7: The thin film absorption spectra for compounds 6, 8, 9 and 10 spun cast from the 10mg/ml CHCl₃ solution.



Figure S8: The solution and thin film absorption spectra for compound 6.



Figure S9: The solution and thin film absorption spectra for compound 8.



Figure S10: The solution and thin film absorption spectra for compound 9.



Figure S11: The solution and thin film absorption spectra for compound 10.

5. CVs of the compounds



Figure S12. First reduction (left) and oxidation (right) cycles of 6, 8, 9 and 10 measured by cyclic voltammetry in dichloromethane solution with tetrabutylammonium hexafluorophosphate (TBAF) electrolyte (0.1 M) at 100 mv/s. the potential is referenced to the Fc/Fc^+ .

6. TGA of the Compounds



Figure S13: Thermal gravimetric analysis (TGA) of **6** (a), **8** (b), **9** (c) and **10** (d) recorded at 10°C/min in a nitrogen atmosphere.

							aThe
Comp.	T_a^a (°C)	charge	$\mu_{aver}{}^{b}(\mathrm{cm}^{2}/\mathrm{Vs})$	$\mu_{max}^{b}(\mathrm{cm}^{2}/\mathrm{Vs})$	$V_{\mathrm{T}}^{c}[\mathbf{V}]$	I_{on}/I_{off}	mal
6	200	Electron	2.6×10 ⁻²	3.2×10 ⁻²	25.6	3.1×10 ⁵	ing
6	220	Electron	3.9×10 ⁻²	4.7×10 ⁻²	25.4	5.2×10 ³	temp
6	240	Electron	4.2×10-2	5.5×10-2	24.8	3.4×10 ³	ratur
6	250	Electron	7.4×10 ⁻²	8.3×10 ⁻²	28.8	5.5×10 ³	tor

7. OFETs characteristics of the compounds Table S1: Summary of the OFETs devices of 6.

^bThe values reported were calculated from ten parallel devices in saturation region; ^c Threshold voltage; ^d Current on/off ratio.



Figure S14: Optimized n-type output curve of compound 6 annealed at 250 °C.

8. Experimental details.



Scheme S1: Synthesis route of BBBT bislactams.



Scheme S2: Synthesis route of BBBT -isoindigo multi-lactams.

- 1 and S1 were purchased from Fluorochem UK.
- 2-decyltetradecyl bromide was synthesized according to the literature. [4]
- **4** was obtained according to the literature. ^[5]

Compound 2.

6-bromoisatin 1 (2.0 g, 8.85 mmol), 2-decyltetradecyl bromide (4.43g, 10.6 mmol), anhydrous potassium carbonate (3.37g, 26.55mmol) in dry DMF (30 ml) and heated at 70 °C under argon for 20 h. After being cooled down to room temperature, water was added to the mixture, extracted with ethyl acetate, the organic fractions washed with brine and dried over MgSO₄. The crude oil was subjected to column chromatography using hexane and dichloromethane (1:2) as eluting to give a yellow oil (3.23g, 65% yield). ¹H NMR (400 MHz, chloroform-d, 300 K), δ (ppm): 7.47 (d, J = 7.9 Hz, 1H), 7.28 (dd, J = 7.9, 1.5 Hz, 1H), 7.04 (d, J = 1.5 Hz, 1H), 3.60 (m, 2H), 1.82-1.87(m, 2H), 1.22-1.43 (m, 40H), 0.88-0.91 (m, 6H). ¹³C NMR (100 MHz, chloroform-d, 300 K), δ (ppm): 182.29, 158.29, 152.29, 133. 46, 126.30, 116.26, 113.99, 44.90, 31.92, 31.47, 31.41, 30.95, 30.08, 29.94, 29.83, 29.69, 29.65, 29.62, 29.57, 29.36, 26.90, 26.90, 26.38, 26.29, 22.70, 14.13, MS (MALDI-TOF, CHCl₃): Calculated for



Figure S15: ¹H NMR of **2** in CDCl₃ at 300K.



Figure S16: ¹³ C NMR of **2** in CDCl₃ at 300K.

Compound 3.

A mixture of 6-bromoisatin **2** (1.0 g, 1.78 mmol), bis(pinacolato)diboron (678 mg, 2.67 mmol), Pd(PPh₃)₂Cl₂ (62 mg, 0.089 mmol) and potassium acetate (349 mg, 3.56 mmol) in anhydrous dioxane (20 mL) was heated at 90 °C for 16 h under argon. The reaction mixture was then cooled down to r.t and quickly plugged through a short pad silica gel with methylene chloride. The collected filtration was concentrated and dried to give crude 6-borate easter isatin, methanol (5 ml) was added and cooled down with dry ice, the methanol solution was filtered and the red viscous **3** was collected and dried (920 mg, 85 %) used without further purification. ¹H NMR (400 MHz, CDCl₃, 300 K), δ (ppm): 7.55 (d, 2H), 7.24 (s, 1H), 3.61 (d, 2H), 1.36 (s, 12H), 1.20-1.29 (m, 40H), 0.85-0.89 (m, 6H). ¹³C NMR (100 MHz, CDCl₃, 300 K), δ (ppm): 184.22, 158.42, 150.46, 130.03, 124.08, 119.34, 115.61, 84.65, 44.67, 35.93, 31.92, 31.52, 31.43, 30.32, 30.20, 30.14, 29.93, 29.78, 29.68, 29.65, 29.63, 29.59, 29.35, 29.34, 26.34. 25.02, 24.87, 22.68, 14.11. MS (LC-MS, CH₃CN): Calculated for C₃₈H₆₄BNO₄, calculated: 609.5, found: 609.3.



Figure S18: ¹³ C NMR of **3** in CDCl₃ at 300K.

To an oven-dried 20 mL microwave vial, 6-borate easter-isatin (**3**) (800 mg, 1.31 mmol), Pd(PPh₃)₄ (20 mg, 0.018 mmol), **4** (130 mg, 0.36 mmol), the tube was sealed, then toluene (6 mL) and 2M K₂CO₃ (3 mL) were added. The mixture was degassed under Argon for half an hour, and then the argon inlet was removed. The tube was subjected to heat at 90 °C for 18 h. After being cooled down to room temperature, the reaction mixture was extracted with EA, and the organic phase was collected and dried with magnesium sulphate, solvent was removed by the reduced pressure, purified by column chromatography (eluent: DCM: EA=5:1) to afford a yellow solid **5** (201 mg, 48 %). ¹H NMR (400 MHz, CDCl₃, 300 K), δ (ppm): 8.21 (s, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.23 (dd, J = 7.6, 1.3 Hz, 1H), 7.01 (d, J = 1.4 Hz, 1H). 3.62-3.68 (m, 4H), 2.52 (s, 6H), 1.89-1.93 (t, 2H), 1.25-1.44 (m, 80H), 0.87-0.91 (m, 12H). ¹³C NMR (100 MHz, CDCl₃, 300 K), δ (ppm): 182.60, 158.19, 151.98, 147.85, 145.84, 139.20, 126.14, 125.99, 124.26, 117.69, 110.68, 45.22, 41.82, 36.24, 31.91, 31.54, 30.05, 29.93, 29.68, 29.64, 29.58, 29.34, 26.47, 26.34, 26.31, 24.87, 22.68, 14.11. MS (MALDI-TOF, CHCl₃): Calculated for C₇₂H₁₁₂N₂O₆S₂: 1164.7962: [M+H]⁺, found: 1165.9.



Figure S19: ¹H NMR of **5** in CDCl₃ at 300K.



Figure S20: ¹³ C NMR of **5** in CDCl₃ at 300K.

5 (200 mg, mmol) was stirred with Eaton's reagent (4 mL) at room temperature in the dark for 3 days. The mixture was poured into ice–water, extracted with chloroform and the organic phase was dried with MgSO₄, the solvent was removed by reduced pressure and the crude product was dried in vacuum, which was followed to be dissolved in pyridine (8 mL) and then the mixture was refluxed overnight. After the mixture was cooled to room temperature, the solvent was removed by reduced pressure and then chloroform was added, retracted with diluted hydrochloride acid, the separated organic phase was dried over MgSO₄, and solvent was removed by reduced pressure again. The crude was purified by column chromatography on silica gel (eluent: CHCl₃) to afford a brown solid **6** (67 mg, 35%). Mp: 232–236 °C; ¹H NMR (400 MHz, CDCl₃, 300 K), δ (ppm): 8.63 (s, 2H), 8.13 (s, 2H), 7.60 (s, 2H), 3.78-3.80 (m, 4H), 2.06 (t, 2H), 1.25-1.46 (m, 80H), 0.86-0.90 (m, 12H). ¹³C NMR (100 MHz, CDCl₃, 300 K), δ (ppm): 182.92, 158.65, 147.88, 141.42, 139.48, 135. 47, 135.18, 120.91, 118.16, 117.16, 102.86, 45.08, 35.92, 31.92, 31.58, 30.02, 29.77, 29.69, 29.65, 29.36, 26.47, 22.69, 14.13. MS (MALDI-TOF, CHCl₃): Calculated for C₇₀H₁₀₄N₂O₄S₂: 1100.74: found: 1100.8. UV-vis (CHCl₃): λ_{max}/nm (ε/M⁻¹ cm⁻¹) = 418 (36800).



Figure S21: ¹H NMR of **6** in CDCl₃ at 300K.



Figure S22: ¹³ C NMR of **6** in CDCl₃ at 300K.



Figure S23: MALDI-TOF of 6.

Compound S2

S2 was obtained from the same procedure with 2 expect Isatin S1 was used as the starting material.

Compound 7

A mixture of N_2H_4 . H_2O (4 ml) and **S2** (300 mg, 0.62 mmol) was heated at 140 °C for 3 days. After being cooled down to room temperature, the mixture was subsequently extracted with ethyl acetate. Organic fractions were combined and washed with brine and dried over MgSO₄ to give a yellow crude oil that was purified by silica column chromatography using dichloromethane as yellow oil (276 mg, yield 92 %).

¹H NMR (400 MHz, Chloroform-d, 300K), δ (ppm): 7.26-7.30 (td, J = 7.7 Hz, 2H), 7.04 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 3.61 (d, J = 7.4 Hz, 2H), 3.55 (s, 2H), 1.90-1.87 (m, 1H), 1.41–1.22 (m, 40H), 0.92-0.89 (m, 6H). ¹³C NMR (101 MHz, Chloroform-d, 300K), δ (ppm): 175.29, 145.11, 127.72,

124.64, 121.98, 108.58, 44.54, 36.05, 35.77, 31.93, 31.62, 30.01, 29.86, 29.68, 29.65, 29.60, 29.36, 26.51, 22.70, 14.13. MS (ESI), Calculated C₃₂H₅₅NO, 469.4284, found: [M+H]⁺: 470.4358.



Figure S24: ¹H NMR of 7 in CDCl₃ at 300K.



Figure S25: ¹³ C NMR of 7 in CDCl₃ at 300K.

Compound 8

Compound **6** (98 mg, 0.09 mmol), **7** (35 mg, 0.075 mmol) and PTSA.H₂O (5 mg, 0.6 equiv) were mixed in toluene (4 mL), the mixture was heated at 120 °C for 24 h. After being cooled down to room temperature, methanol was added, the solid was filtered and collected, further purified by the column chromatography on silica gel (eluent, PE: CHCl₃ =1:2) to afford solid **8** (65 mg, yield: 56 %, calculated based on the **7**), and **9** (10 mg, yield: 7 %, calculated based on the **7**). Mp: 130 –134 °C; ¹H NMR (400

MHz, TCE-D₂, 300K), δ (ppm): 9.79 (s, 1H), 9.11 (d, J = 8.0 Hz, 1H), 8.54 (s, 1H), 8.47 (s, 1H), 8.01 (s, 1H), 7.51 (s, 1H), 7.40 (s, 1H), 7.38 (t, J = 7.8 Hz, 1H), 7.03 (t, J = 7.8 Hz, 1H), 6.81 (d, J = 7.9 Hz, 1H), 3.83 – 3.69 (m, 6H), 2.08 – 1.90 (m, 4H), 1.51 – 1.11 (m, 171H), 0.83-0.89 (m, 24H). ¹³C NMR (101 MHz, TCE-D₂, 300K), δ (ppm): 183.01, 168.08, 167.66, 158.77, 147.50, 145.02, 142.65, 141.79, 138.89, 136.10, 134.67, 134.04, 133.96, 132.31, 129.71, 122.77, 121.35, 117.38, 108. 31, 102.69, 44.51, 36.08, 31.82, 31.52, 31.45, 29.98, 29.62, 29.57, 29.27, 26.43, 26.33, 22.63, 14.16. MS (MALDI-TOF, CHCl₃): C₁₀₂H₁₅₇N₃O₄S₂, calculated: 1552.16, found: 1552.4. UV-vis (CHCl₃): λ_{max}/nm ($\varepsilon / M^{-1} cm^{-1}$) = 462 nm (36400).



Figure S26: ¹H NMR of **8** in TCE-D₂ at 300K.



Figure S27: 13 C NMR of 8 in TCE-D₂ at 300K.



Figure S28: Partial ¹³ C NMR spectra of **8** in TCE-D₂ at 300K.



Figure S29: MALDI-TOF of 8.

Compound **6** (50 mg, 0. 045 mmol), **7** (56 mg, 0.12 mmol) and PTSA.H₂O (8 mg, 0.05 mmol) were mixed in toluene (3 mL), the mixture was refluxed overnight, after being cooled down to room temperature, methanol was added, the solid was filtered and collected, further purified by the column chromatography on silica gel (eluent, PE: CHCl₃ =1:1) to afford violet solid **9** (55 mg, 62 %). Mp: 125 –129 °C; ¹H NMR (400 MHz, TCE-D₂, 300K), δ (ppm), 9.69 (s, 2H), 9.12 (d, *J* = 7.9 Hz, 2H), 8.39 (s, 2H), 7.37 (s, 2H), 7.34 (t, 2H), 7.04 (t, *J* = 7.8 Hz, 2H), 6.76 (d, *J* = 7.8 Hz, 2H), 3.64-3.82 (m, 8H), 1.88-2.10 (m, 6H), 1.22 –1.32(m, 160H), 0.84-0.88 (m, 24 H). ¹³C NMR (101 MHz, TCE-D₂, 300K), δ (ppm): 168.04, 167.78, 144.89, 142.59, 138.29, 136.58, 134.98, 133.65, 133.30, 132.62, 132.36, 129.53, 124.18, 122.26, 121.93, 121.44, 115.59, 108. 24, 100.14, 44.73, 44.43, 36.09, 35.93, 31.83, 31.54, 30.04, 29.98, 29.93, 29.63, 29.58, 29.28, 26.49, 26.44, 22.64, 14.48, 14.16. MS (MALDI-TOF, CHCl₃):

Calculated for $C_{134}H_{210}N_4O_4S_2$, calculated: 2003.5794, found for: 2003.4, UV-vis (CHCl₃): $\lambda_{max}/nm (\epsilon / M^{-1} cm^{-1}) = 492 nm (56100)$.



Figure S30: ¹H NMR of **9** in TCE-D₂ at 300K.



Figure S31: 13 C NMR of **9** in TCE-D₂ at 300K.



Figure S32: Partial zoomed in ¹³C NMR spectra of the alkyl chain region of **9** in TCE-D₂ at 300K.



Figure S33: MALDI-TOF of 9.

A solution of hexaethyltriaminophosphine (7.95 mg, 0.029mmol, 1.0 equiv.) in DCM (1 mL) was added dropwise to a solution of **8** (45 mg, 0.029 mmol, 1.0 equiv.) in DCM (3 mL) at -78°C. The reaction mixture was then allowed to warm to room temperature overnight. The reaction mixture was evaporated under reduced pressure to dryness and the residue was washed with ethyl acetate and methanol, the solid was filtered and dried under reduced pressure to give the violet product **10** (40 mg, 92%). Mp: 290 – 294 °C; ¹H NMR (400 MHz, TCE-D₂, 403K), δ (ppm): 9.90 (s, 1H), 9.84 (s, 1H), 9.21 (d, *J* = 7.7 Hz, 2H), 8.40 (s, 1H), 8.37 (s, 1H), 7.46 (s, 1H), 7.42 (s, 1H), 7.30 (t, *J* = 7.9 Hz, 2H), 6.98 (t, *J* = 7.7 Hz, 2H), 6.79 (d, *J* = 7.8 Hz, 2H), 4.00-4.02 (m, 4H), 3.93-3.94 (m, 4H), 3.78-3.80 (m, 4H), 2.07-2.29

(m, 6H), 1.32- 1.65 (m, 240H), 0.93- 0.97 (m, 36H).). ¹³C NMR (101 MHz, TCE-D₂, 403K), δ (ppm): 168.14, 167.89, 145.35, 144.47, 143.07, 138.49, 136.59, 136.54, 135.12, 133.73, 133.64, 135.12, 133.73, 133.64, 132.33, 129.95, 122.69, 121.85, 121.62, 115.18, 109.70, 107.75, 99.90, 45.43, 45.25, 45.01, 36.44, 31.59, 29.90, 29.87, 29.79, 29.36, 29.31, 28.96, 26.68, 26.62, 26.52, 22.26, 13.56. MS (MALDI-TOF, CHCl₃): Calculated for C₂₀₄H₃₁₄N₆O₆S₄, 3072.3333, found: 3072.0. UV-vis (CHCl₃): λ_{max}/mm ($\epsilon / M^{-1} cm^{-1}$) = 514 nm (87300).



Figure S34: ¹H NMR of **10** in TCE-D₂ at 403K.



Figure S35: 13 C NMR of **10** in TCE-D₂ at 403K.



Figure S36: Partial zoomed in ¹³C NMR spectra of the alkyl chain region of **10** in TCE-D₂ at 403K.



Figure S37: MALDI-TOF of 10.

9. References

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