

Electronic Supplementary Information

Structure –property relationships in multifunctional thieno(bis)imide-based semiconductors with different sized and shaped N-alkyl ends

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1.0 Synthesis

General procedure for the synthesis of thienoimides **4a-g**.

A solution of thieno[2,3-*c*]furan-4,6-dione (1.54 g, 1 mmol) **2** and alkylamine **3** (1.5 mmol) in 10 ml of toluene was refluxed for 48 h then the solvent was removed. The solid so obtained (made by a mixture of the regioisomers 2-(alkylcarbamoyl)thiophene-3-carboxylic acid and 3-(alkylcarbamoyl)thiophene-2-carboxylic acid), was washed with pentane and used for the following intramolecular dehydration without further purification. The isomers mixture (7.13 mmol) in thionyl chloride (140 ml) was refluxed for 5 h after that SOCl₂ was removed by distillation. The crude so obtained was purified by flash chromatography on silica gel to afford compounds **4a-g**.

*5-Methyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **4a**: Flash chromatography on silica gel, by using petroleum ether/CH₂Cl₂/AcOEt 80:10:10 as eluting phase afforded compound **4a** as a pale beige solid (Y = 91%).

EI-MS m/z 167 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.74 (d, ³J = 4.8 Hz, 1H), 7.30 (d, ³J = 4.8 Hz, 1H), 3.11 (s, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.0, 162.8, 144.8, 140.9, 137.3, 121.1, 24.3.

*5-Propyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **4b**: Flash chromatography on silica gel, by using petroleum ether/AcOEt 90:10 as eluting phase afforded compound **4b** as a pale beige solid (Y = 92%).

EI-MS m/z 195 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.74 (d, ³J = 4.8 Hz, 1H), 7.30 (d, ³J = 4.8 Hz, 1H), 3.57 (t, 2H), 1.67 (m, 2H), 0.94 (t, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.0, 162.8, 144.7, 140.9, 137.2, 121.1, 40.1, 22.1, 11.3.

*5-Hexyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **4d**: Flash chromatography on silica gel, by using petroleum ether/AcOEt 90:10 as eluting phase afforded compound **4d** as a yellow oil (Y > 95 %).

EI-MS m/z 237 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.74 (d, ³J = 4.8 Hz, 1H), 7.29 (d, ³J = 4.8 Hz, 1H), 3.59 (t, 2H), 1.64 (m, 2H), 1.31 (m, 6H), 0.88 (t, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.0, 162.8, 144.7, 140.9, 137.2, 121.1, 38.5, 31.4, 28.8, 26.5, 22.5, 14.0.

*5-Cyclohexyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **4e**: Flash chromatography on silica gel, by using petroleum ether/AcOEt 95:5 as eluting phase afforded compound **4e** as a white solid (Y = 83 %).

EI-MS m/z 235 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.71 (d, ³J = 4.8 Hz, 1H), 7.27 (d, ³J = 4.8 Hz, 1H), 3.99 (m, 1H), 2.13 (m, 2H), 1.77 (m, 2H), 1.74 (m, 3H), 1.33 (m, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.0, 162.8, 144.5, 140.9, 137.0, 121.0, 51.3, 30.1, 26.0, 25.0.

5-2-ethylhexyl-4H-thieno[2,3-c]pyrrole-4,6(5H)-dione, **4f**: Flash chromatography on silica gel, by using petroleum ether/Et₂O 90:10 as eluting phase afforded compound **4f** as a yellow oil (Y = 86 %).

EI-MS *m/z* 265 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.74 (d, ³J = 4.8 Hz, 1H), 7.30 (d, ³J = 4.8 Hz, 1H), 3.49 (d, ³J = 7.2, 2H), 1.78 (m, 1H), 1.30 (m, 8H), 0.89 (m, 6H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.5, 163.3, 144.9, 137.5, 137.3, 121.6, 121.1, 42.6, 38.5, 30.7, 28.7, 24.0, 23.2, 14.3, 10.7.

5-Octyl-4H-thieno[2,3-c]pyrrole-4,6(5H)-dione, **4g**: Flash chromatography on silica gel, by using petroleum ether/AcOEt 90:10 as eluting phase afforded compound **4g** as a yellow oil (Y = 67 %).

EI-MS *m/z* 265 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.34 (d, ³J = 4.8 Hz, 1H), 7.30 (d, ³J = 4.8 Hz, 1H), 3.60 (t, 2H), 1.64 (m, 2H), 1.29 (m, 10H), 0.87 (t, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 164.0, 162.8, 144.7, 140.9, 137.2, 121.1, 38.5, 31.8, 29.2, 28.8, 26.8, 22.6, 14.1.

General procedure for the synthesis of brominated compounds 5a-g.

Thienoimide **4a-g** (1.41 mmol) was dissolved in trifluoroacetic acid (6 ml). After external ice cooling, 1 ml of concentrated sulfuric acid was introduced into the reactor. To this mixture solid N-bromosuccinimide (NBS, 1.37 mmol) was added in small portions over 6 h. After stirring overnight at room temperature, the brown solution was diluted with 10 ml of water and extracted with dichloromethane. The organic phase was dried over anhydrous magnesium sulfate and evaporated. The crude so obtained was then purified by flash chromatography on silica gel to afford compounds **5a-g**.

2-Bromo-5-methyl-4H-thieno[2,3-c]pyrrole-4,6(5H)-dione, **5a**: Purification by flash chromatography by using silica gel and petroleum ether/CH₂Cl₂/AcOEt = 80:10:10 as eluent afforded **5a** as a white solid in 67% yield.

EI-MS *m/z* 247 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.31 (s, 1H), 3.09 (s, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 163.0, 162.0, 125.5, 123.8, 24.5.

2-Bromo-5-propyl-4H-thieno[2,3-c]pyrrole-4,6(5H)-dione, **5b**: Purification by flash chromatography by using silica gel and petroleum ether/AcOEt = 90:10 as eluent afforded **5b** as a white solid in 89% yield.

EI-MS *m/z* 275 (M⁺). ¹H NMR (CDCl₃, TMS/ppm) δ 7.31 (s, 1H), 3.55 (t, 2H), 1.66 (m, 2H), 0.93 (t, 3H). ¹³C NMR (CDCl₃, TMS/ppm) δ 163.0, 162.0, 143.8, 140.4, 125.4, 123.8, 40.2, 22.0, 11.2.

2-Bromo-5-hexyl-4H-thieno[2,3-c]pyrrole-4,6(5H)-dione, **5d**: Purification by flash chromatography by using silica gel and petroleum ether/AcOEt/CH₂Cl₂ = 90:5:5 as eluent afforded **5d** as yellow oil in 84% yield.

EI-MS m/z 317 (M^+). ^1H NMR (CDCl_3 , TMS/ppm) δ 7.30 (s, 1H), 3.57 (t, 2H), 1.62 (m, 2H), 1.30 (m, 6H), 0.88 (t, 3H). ^{13}C NMR (CDCl_3 , TMS/ppm) δ 163.0, 162.0, 143.9, 140.5, 125.4, 123.8, 38.7, 31.3, 28.7, 26.4, 22.5, 14.0.

*2-Bromo-5-cyclohexyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **5e**: Purification by flash chromatography by using silica gel and petroleum ether/AcOEt = 95:5 as eluent afforded **5e** as a yellow oil in 79% yield.

EI-MS m/z 315 (M^+). ^1H NMR (CDCl_3 , TMS/ppm) δ 7.28 (s, 1H), 3.97 (m, 1H), 2.11 (m, 2H), 1.85 (m, 2H), 1.70 (m, 3H), 1.30 (m, 3H). ^{13}C NMR (CDCl_3 , TMS/ppm) δ 163.0, 162.0, 143.7, 140.5, 125.1, 123.7, 51.6, 30.0, 26.0, 25.0.

*2-Bromo-5-ethylhexyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **5f**: Purification by flash chromatography by using silica gel and petroleum ether/AcOEt = 95:5 as eluent afforded **5f** as dark white solid in 78% yield.

EI-MS m/z 345 (M^+). ^1H NMR (CDCl_3 , TMS/ppm) δ 7.31 (s, 1H), 3.48 (d, $^3J = 7.2$ Hz, 2H), 1.76 (m, 1H), 1.28 (m, 8H), 0.89 (m, 6H). ^{13}C NMR (CDCl_3 , TMS/ppm) δ 163.2, 162.2, 143.8, 125.4, 124.0, 123.6, 42.5, 38.3, 30.4, 28.4, 23.7, 22.9, 14.0, 10.4.

*2-Bromo-5-octyl-4H-thieno[2,3-*c*]pyrrole-4,6(5H)-dione*, **5g**: Purification by flash chromatography by using silica gel and petroleum ether/AcOEt/ CH_2Cl_2 90:5:5 as eluent afforded **5g** as white solid in 88% yield.

EI-MS m/z 345 (M^+). ^1H NMR (CDCl_3 , TMS/ppm) δ 7.30 (s, 1H), 3.57 (t, 2H), 1.62 (m, 2H), 1.27 (m, 10H), 0.87 (t, 3H). ^{13}C NMR (CDCl_3 , TMS/ppm) δ 163.0, 162.0, 143.9, 140.5, 125.4, 123.8, 38.7, 31.8, 29.2, 29.1, 28.7, 26.8, 22.6, 14.1.

1.1 Optical properties in solution

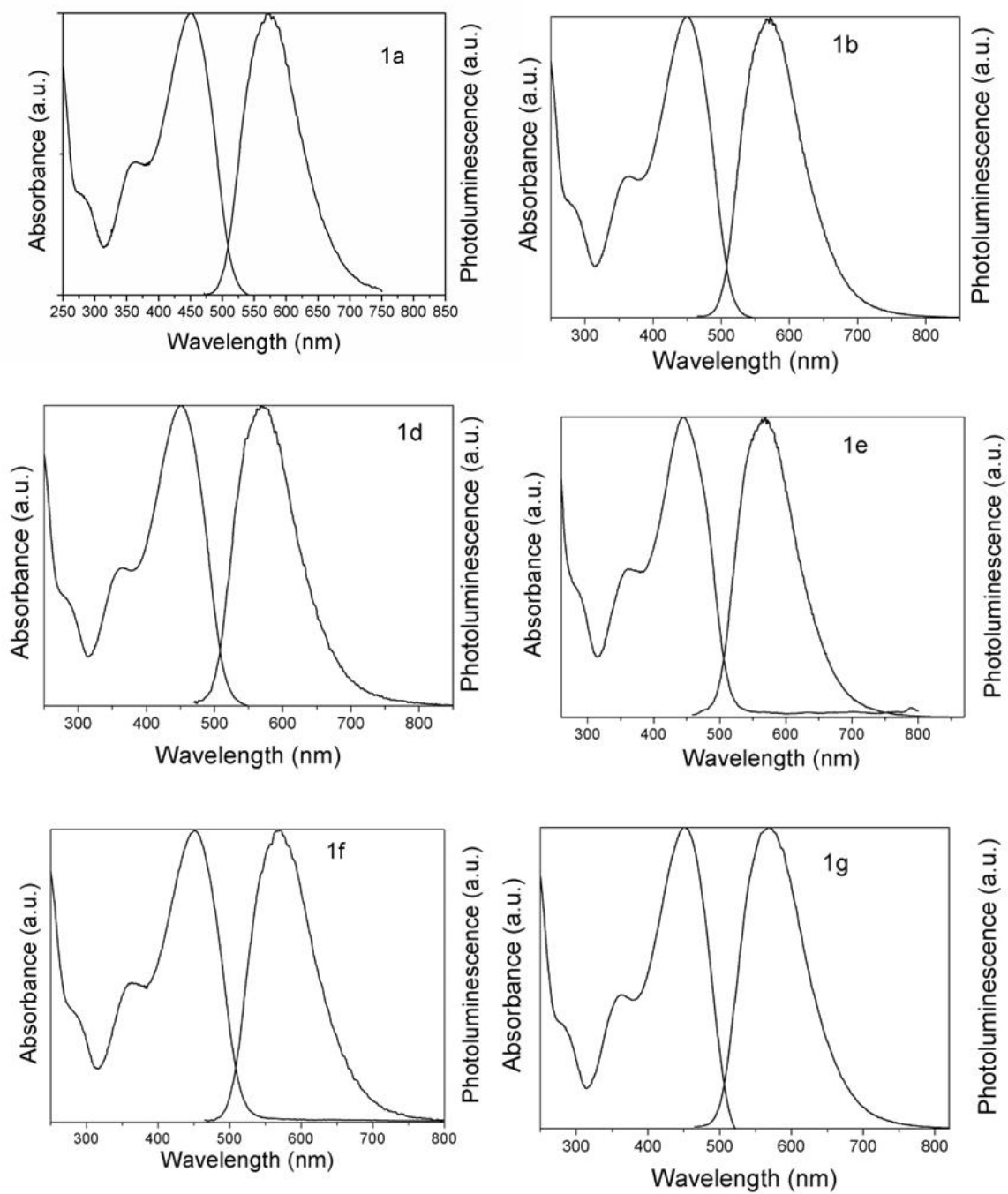


Fig. S1.

| Item | $\lambda_{\text{max,}}$ CH₂Cl₂ (nm) | $\lambda_{\text{em,}}$ CH₂Cl₂ (nm) |
|------------------------|---------------------------------------------------------------------|--------------------------------------------------------------------|
| C1-NT4N (1a) | 451 | 570 |
| C3-NT4N (1b) | 451 | 572 |
| C4-NT4N (1c) | 449 | 572 |
| C6-NT4N (1d) | 451 | 568 |
| C6cyc-NT4N (1e) | 444 | 568 |
| C6br-NT4N (1f) | 451 | 571 |
| C8-NT4N (1g) | 450 | 568 |

Table S1. Optical properties in dilute DCM solution

1.2 Differential Scanning Calorimetry

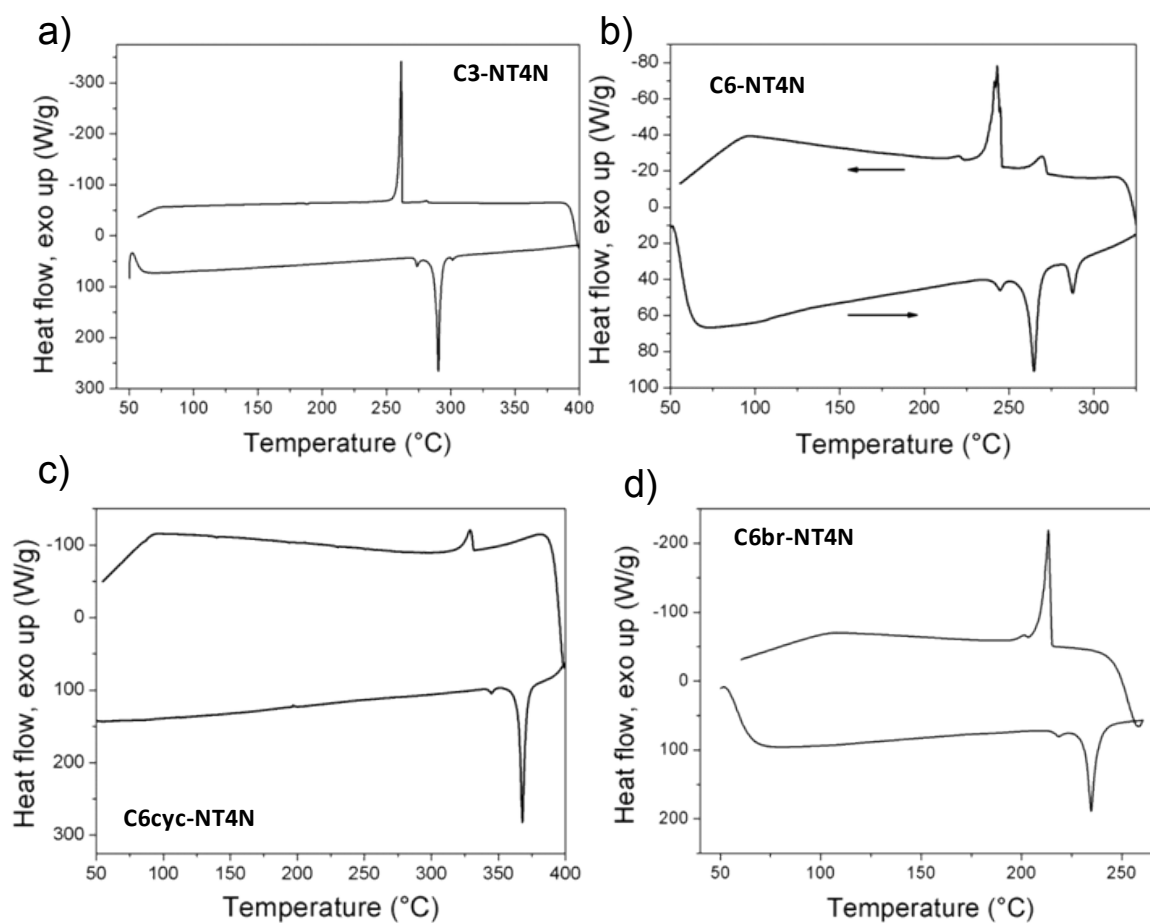


Fig. S2. DSC traces (second heating and cooling steps) at 20°C/min.

1.3 Thin deposits and thermal behaviour

Compound *C1-NT4N*, **1a** formed small crystallites with irregular shape whose mean size was below 2 μm (therefore at the limits of the optical resolution). The crystallites exhibited a slight birefringence disappearing at about 350 °C in air (and at 430 °C when the thin deposit is heated in between two glass slides).

Compound *C3-NT4N*, **1b** formed micrometer sized rod-like crystals. POM showed the typical behaviour of optical anisotropic substances, *i.e.* the crystals appeared coloured under crossed

polars. By rotating the crystal orientation vs. the polarised light, the crystals extinguished in four positions at intervals of 90°. The evidence of light extinguishment at the same orientations in all crystals indicated that all domains have the same orientation. No correlation among the orientation of different crystals was observed. By heating above 260 °C, **1b** became a smectic liquid crystal. At this temperature the size of birefringent domains increased up to few tens µm and then melted at about 300 °C. At this temperature thin deposit dewetted forming a homogeneous distribution of droplets. The liquid droplets have the typical behaviour of smectic LC. When cooling down below LC transition the droplets form large platelet like, highly birefringent crystals.

Compound C4-NT4N, 1c, similarly to C3-NT4N, formed rod-like crystals whose size range from few tens µm to few hundred µm with the same behaviour observed at POM. Each crystal exhibited birefringence that extinguished by crossing the polarisers. A liquid crystal transition occurred at about 270°C to give a smectic phase. Finally, the transition to isotropic phase occurred at 290 °C. When cooled down to room temperature the droplets form large, birefringent, crystals.

Compound C6-NT4N formed a continuous film on the surface whose thickness increases from the centre of thin deposit to the boundaries. The film exhibited birefringence without extinguishing at any direction under POM. Furthermore in the centre of the deposit birefringent fiber-like crystals were often observed. Noticeably AFM showed that the fibers derived from the aggregation of small platelet-like crystals. At 245°C C6-NT4N became a liquid crystal and finally melted at about 300°C. At this temperature thin deposit dewetted forming a homogeneous distribution of droplets. When cooled down to room temperature the droplets formed large, birefringent, crystals.

Compound C6cyc-NT4N, **1e** formed rod-like crystals whose size ranged from few tens μm to few hundred μm . The crystals exhibited birefringence and extinguished when oriented parallel or perpendicular to the polariser. **1e** decomposed at about 400°C in air.

Compound C6br-NT4N, **1f** formed small crystals of irregular shape whose typical size ranged between $2\ \mu\text{m}$ and $10\ \mu\text{m}$. At $210\ ^\circ\text{C}$ it formed a smectic liquid crystal. At this temperature the size of birefringent domains increased until few tens μm . the transition to isotropic liquid occurred at 240°C . When cooled at room temperature the droplets form large platelet like, birefringent crystals.

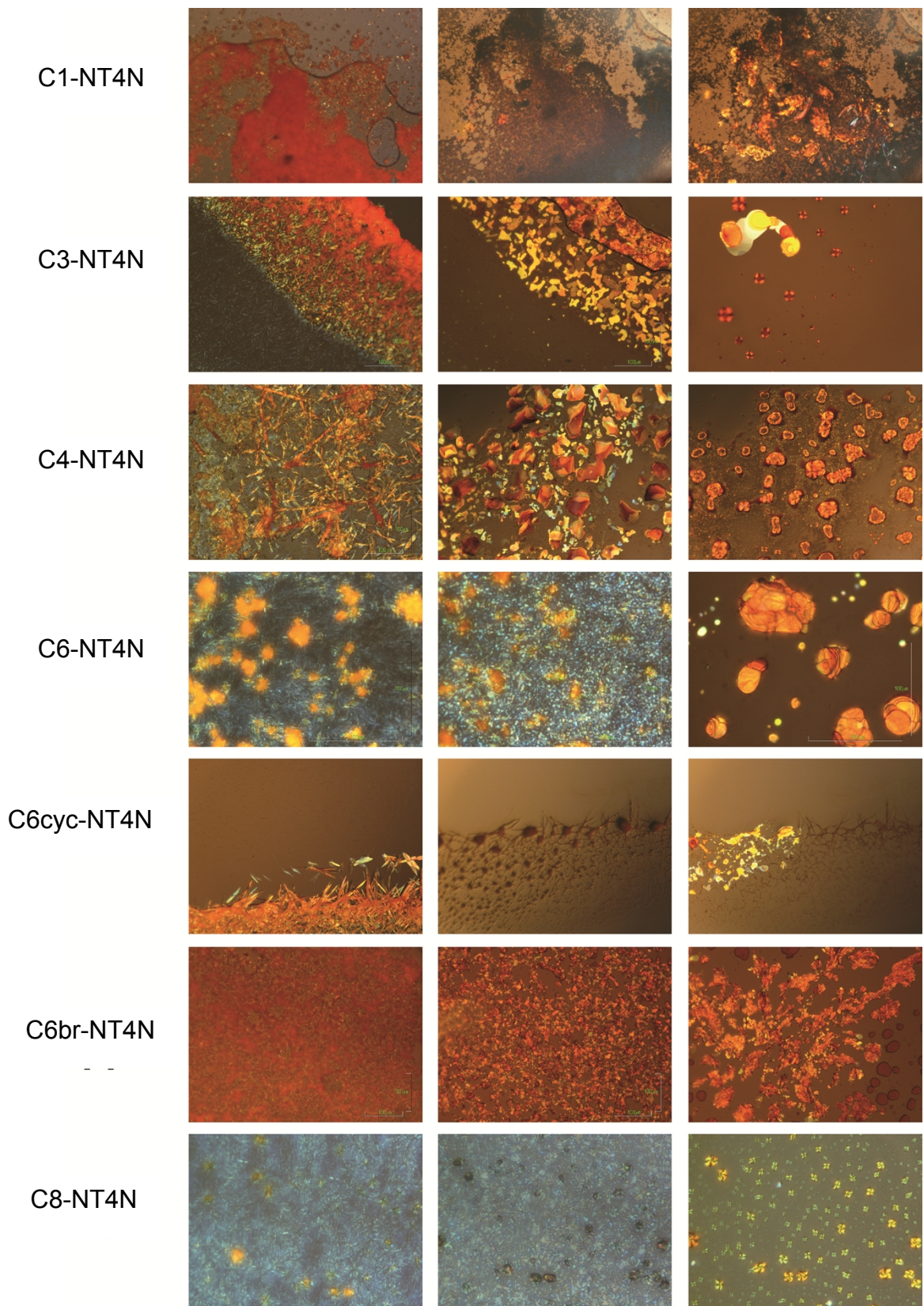


Fig. S3.

1.4 X-ray diffraction

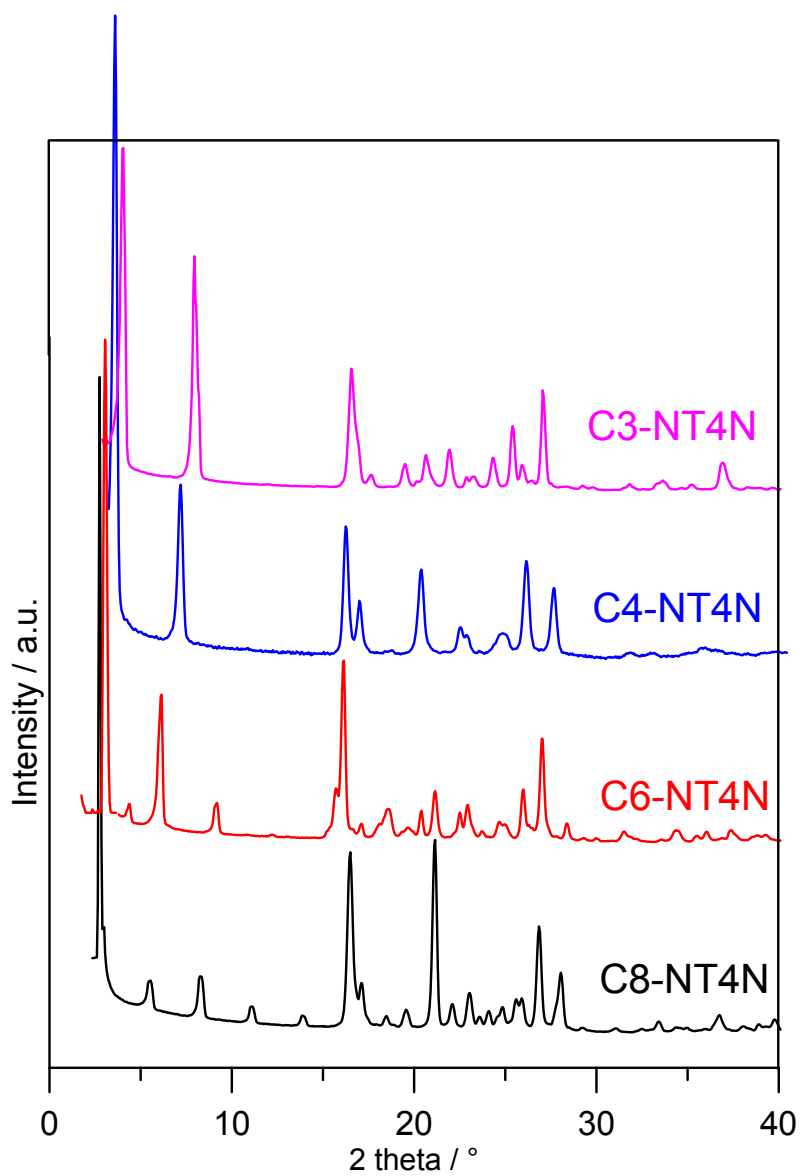


Fig. S4. XRD patterns of compounds C3, C4, C6, C8-NT4N (powders).

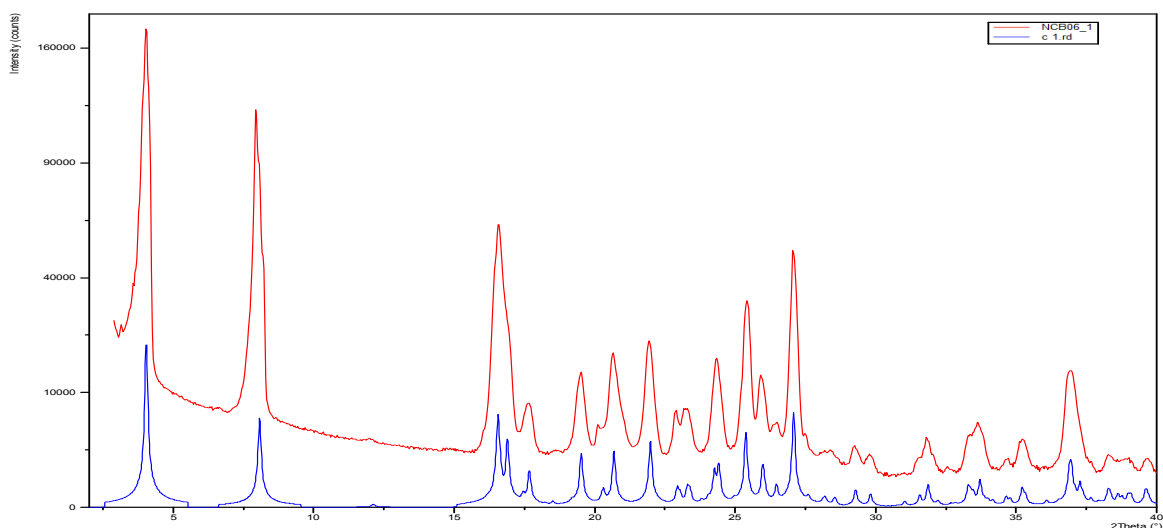


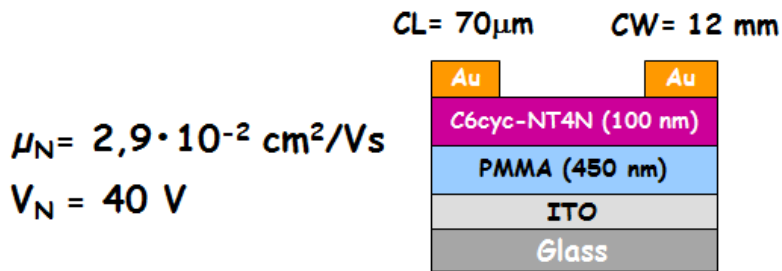
Fig. S5. Comparison between experimental (red line) and calculated (blue) profile for compound C3-NT3N.

Single crystal X-ray diffraction (SC XRD): Crystal data for C3-NT4N were collected on an Oxford Xcalibur S with MoK α radiation, $\lambda = 0.71073 \text{ \AA}$, monochromator graphite at room temperature. Crystal data and structure refinement parameters are summarized for C3-NT4N in the Table below. SHELX97¹ was used for the structure solution and refinement based on F^2 . Non-hydrogen atoms were refined anisotropically. The MERCURY² software package was used for the graphical representation of the structure and powder pattern calculation.³

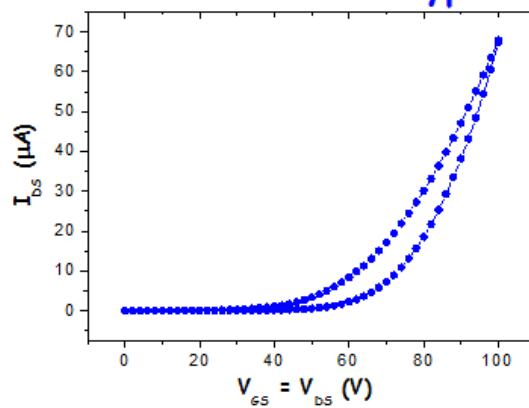
| | |
|---------------------------------------|------------------------------------------------------------------------------|
| Formula | C ₂₆ H ₂₀ N ₂ O ₄ S ₄ |
| M, g mol ⁻¹ | 552.68 |
| Crystal system | Monoclinic |
| Space Group | C2/c |
| <i>a</i> , Å | 7.4707(8) |
| <i>b</i> , Å | 7.7479(6) |
| <i>c</i> , Å | 43.819(6) |
| β , deg | 91.54(1) |
| <i>V</i> , Å ³ | 2535.4(5) |
| <i>Z</i> | 4 |
| Calculated density g cm ⁻³ | 1.448 |
| R_1^a , wR_2^b | 0.0787, 0.1785 |
| <i>GOF on F</i> ² | 1.167 |

a) $R_1 = \sum(|F_o| - |F_c|) / \sum(|F_o|)$ and b) $wR_2 = [\sum\{w(F_o^2 - F_c^2)^2\} / \sum\{w(F_o^2)^2\}]^{1/2}$

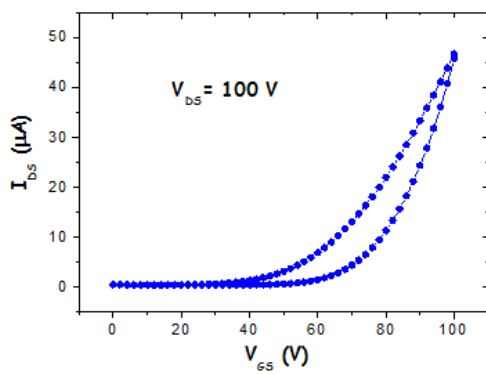
1.5 Electrical properties of compound C6cyc-NT4N



Locus curve N type



Saturation Transfer curve N type



Multiple Output curve N type

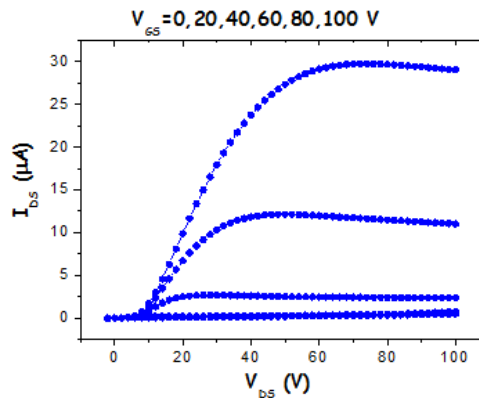
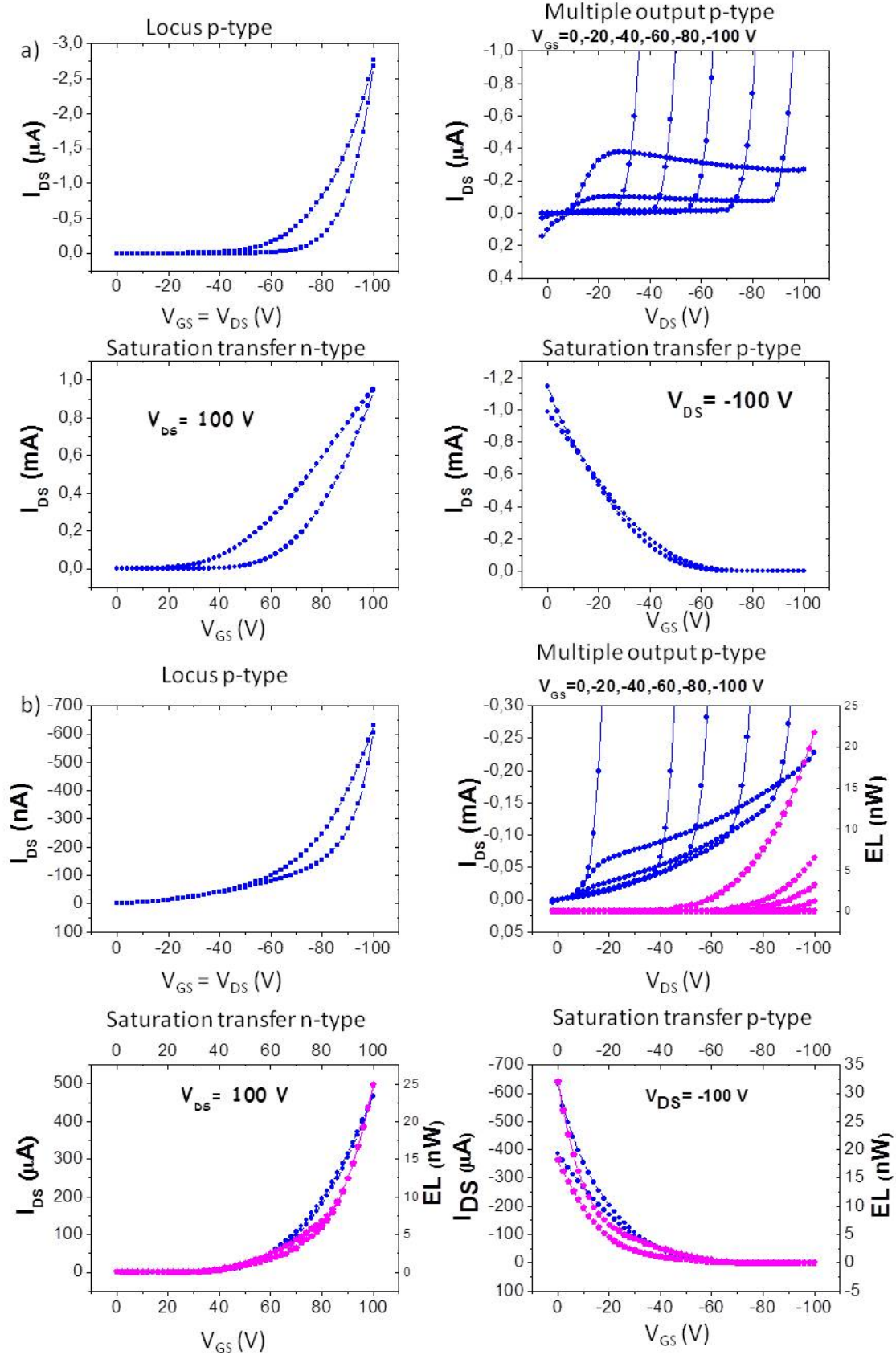


Fig. S6.

1.6 Locus p-type, multiple output p-type and saturation transfer curves



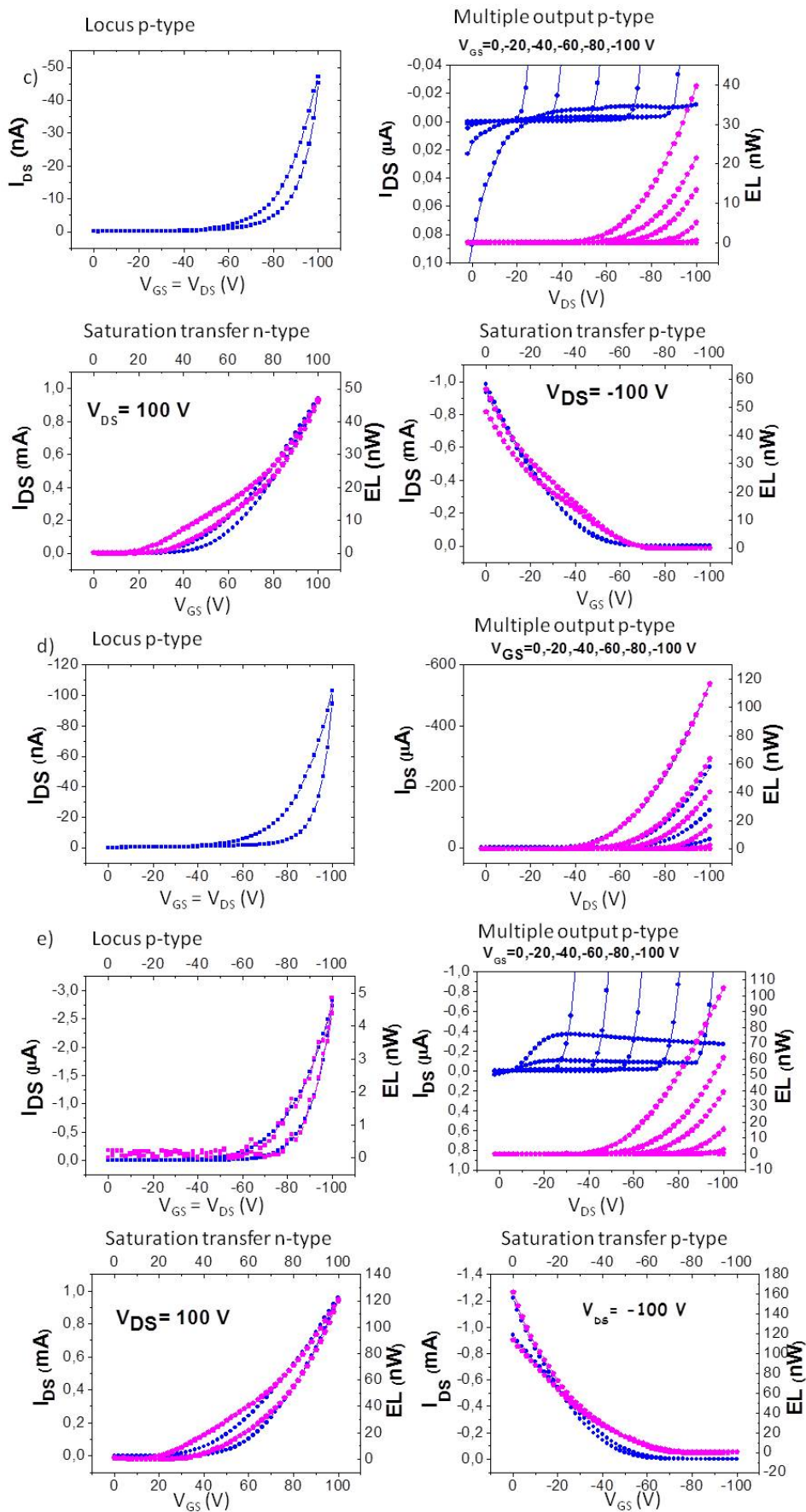


Fig. S7. Electrical responses for compounds C1-NT4N (a), C3-NT4N (b), C4-NT4N (c), C6-NT4N (d) and C8-NT4N (e).

1.7 Locus n-type, multiple output n-type and saturation transfer curves

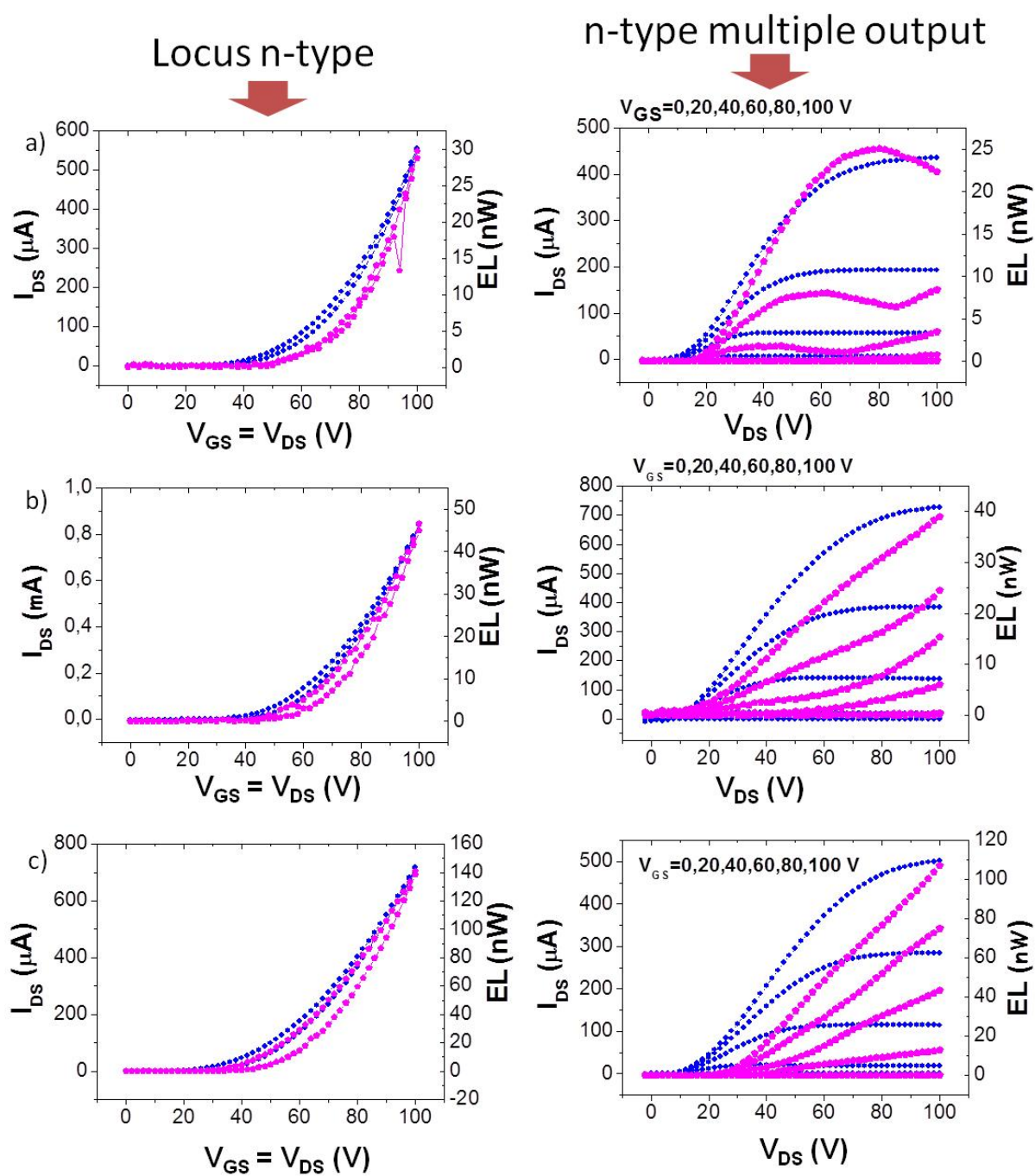


Fig. S8. Electrical responses for compounds C3-NT4N (a), C4-NT4N (b), C6-NT4N (c).

1.8 Computational Details

Density functional theory (DFT) calculations were carried out with the CRYSTAL09 package.^{4,5} The exchange-correlation contributions to the total energy were treated using the hybrid B3LYP functional^{6,7} with 20% of exact Hartree-Fock exchange that has shown a better agreement with experiments in calculated geometries and vibration frequencies than other functionals (e.g. LDA and GGA).^{8,9}

The all-electron Gaussian-type basis sets adopted were 6-31(d1) for oxygen,¹⁰ nitrogen¹¹ and carbon,¹² 31(p1) for hydrogen¹⁰ and 8-6311(d1) for sulphur.¹³ The condition for SCF convergence was set to 10^{-7} and 10^{-10} hartree during geometry optimization and frequency calculation, respectively. In the geometry optimization process the threshold for the maximum and the root-mean-square (RMS) forces and the maximum and the RMS atomic displacements on all the atoms have been set to 0.000450 and 0.000300 a.u. and 0.001800 and 0.001200 a.u., respectively.

Long-range dispersion interactions, of primary importance in molecular crystals, are accounted by a post-DFT dispersive contribution, suggested by Grimme,¹⁴ to the computed ab initio total energy and gradients. Such correction has been recently implemented in the CRYSTAL code and has been successfully validated in particular in combination with the B3LYP functional.^{15,16} Van der Waals radii and dispersion coefficients C_6 were taken from Table 1 of reference ¹⁷.

Vibrational frequencies, within harmonic approximation, were calculated on the optimized molecule geometry by diagonalising the mass-weighted Hessian matrix W_{ij}

$$W_{ij}(\Gamma) = \sum_G \frac{H_{ij}^{0G}}{\sqrt{M_i M_j}} \quad (1)$$

where H_{ij}^{0G} is the Hessian matrix of second derivatives of the electron+nuclear repulsion energy E evaluated at equilibrium, with respect to the displacement coordinates u_i and u_j of atom A in cell 0 and of atom B in cell G, respectively:

$$\sum_G H_{ij}^{0G} = \sum_G \left[\frac{\partial^2 E}{\partial u_i^0 \partial u_j^G} \right]_0, \quad i = 1, \dots, 3N; \quad j = 1, \dots, 3N \quad (2)$$

The Hessian matrix is obtained by numerical differentiation of analytical first derivatives $v_j = \partial E / \partial u_j$ using a difference quotient or “two point” formula^{5,18}

$$h(x) = \frac{[v_j(x + u_i) - v_j(x)]}{u_i} \quad (3)$$

with a step $u_i = 0.001\text{\AA}$.

The intramolecular reorganization energy λ_i has been evaluated within the adiabatic potential (AP) approach.¹⁹ according to the following equation:

$$\lambda_i = E_n(n) - E_n(c) + E_c(c) - E_c(n) \quad (4)$$

where the total electronic energy E subscripts and brackets indicate the charge state and the equilibrium geometry of the neutral (n) and charged (c) molecule, respectively.

In Table S2, all the computed values of λ_i are reported.

| Molecule | λ_i^h [meV] | λ_i^e [meV] |
|--------------------|---------------------|---------------------|
| C1-NT4N | 321 | 328 |
| C3-NT4N | 319 | 333 |
| C4- NT4N | 318 | 337 |
| C6- NT4N | 342 | 351 |
| C8- NT4N | 341 | 350 |
| C6cyc- NT4N | 346 | 366 |
| C6br- NT4N | 330 | 349 |

Table S2. Calculated intramolecular reorganization energy, λ_i , by adiabatic potential surfaces of the neutral, cation and anion species.

The charge transfer integral τ is evaluated for the nearest neighboring molecules through the diabatic model^{20,21}:

$$\tau = \langle \Phi_{FO}^{0,site1} | H | \Phi_{FO}^{0,site2} \rangle \quad (5)$$

$\Phi_{FO}^{0,site1}$ and $\Phi_{FO}^{0,site2}$ represent the frontier orbitals (i.e. HOMO or LUMO) of isolated molecules 1 and 2, respectively and H is the electronic Hamiltonian for a non-interacting dimer pair. Here, τ has been estimated through the application of Koopmans' theorem in the energy-splitting in dimer (ESID) model²². The charge transfer integrals for hole, τ_h , and for electron, τ_e , transport are computed as half the energetic differences between HOMO and HOMO-1 and between LUMO and LUMO+1 energy levels of a molecular dimer, respectively.

We assumed the non-adiabatic hopping model and we computed the transfer rate constants k_{CT} according to the Marcus-Levich-Jortner formulation^{23,24}:

$$k_{CT} = \frac{2\pi}{\hbar} \tau^2 \frac{1}{\sqrt{4\pi\lambda_o k_B T}} \sum_{v=0}^{\infty} \left[\exp(-S_{eff}) \frac{S_{eff}^v}{v!} \exp\left(-\frac{(\Delta G^0 + \lambda_o + v\omega_{eff})^2}{4\lambda_o k_B T}\right) \right] \quad (6)$$

Here, ΔG^0 is assumed zero for the self-exchange process (i.e. $M^0 + M^c \leftrightarrow M^c + M^0$, for molecule M in neutral and charged states 0 and c, respectively). The quantum description of normal modes is included through an effective frequency ω_{eff} defined by the following equation:

$$\omega_{eff} = \sum_m \omega_m \frac{S_m}{\sum_n S_n} \quad \omega_{eff} = \sum_m \omega_m \frac{S_m}{\sum_n S_n} \quad (7)$$

The summation runs over all the vibrational normal modes m of frequencies ω_m , and S_m denotes the Huang–Rhys (HR) factor measuring charge-phonon coupling strength. The latter can be obtained from the dimensionless displacement parameter B_k :

$$S_k = \frac{1}{2} B_k^2 \quad (8)$$

that, in the harmonic approximation, is defined as:

$$B_k = \sqrt{\frac{\omega_k}{\hbar}} \{X_q - X_p\} M^{0.5} L_k(q) \quad (9)$$

where X_q and X_p are the equilibrium Cartesian coordinates of the q and p charge states, respectively, M is the $3N \times 3N$ diagonal matrix of the atomic masses, and $L_k(q)$ is the $3N$ vector describing the normal coordinate Q_k of the q charge state in terms of mass-weighted Cartesian coordinates.

From Eq (7) the effective Huang-Rhys factor S_{eff} is derived:

$$S_{eff} = \frac{\lambda_i}{\hbar \omega_{eff}} \quad S_{eff} = \frac{\lambda_i}{\hbar \omega_{eff}} \quad (10)$$

The outer-sphere reorganization energy λ_o in Eq. (10) has been taken as a parameter equal to 0.1 eV, in agreement with recent studies. The bulk charge mobility has been computed assuming a Brownian motion of the charge carrier, described by the following diffusion coefficient D :

$$D = \frac{1}{6} \sum_n (r_n)^2 k_{CT,n} P_n \quad D = \frac{1}{6} \sum_n (r_n)^2 k_{CT,n} P_n \quad (11)$$

where n runs over all the possible hopping pathways (v. Table 5) and P_n is the probability associated with the hopping defined as follows:

$$P_n = \frac{k_{CT,n}}{\sum_j k_{CT,j}} \quad P_n = \frac{k_{CT,n}}{\sum_j k_{CT,j}} \quad (12)$$

Finally the bulk charge mobility μ is obtained from the Einstein equation:

$$\mu = \frac{eD}{k_B T} \quad \mu = \frac{eD}{k_B T} \quad (13)$$

All the calculated charge transport data for molecule C3-NT4N are reported in Table S3.

| | ω_{eff} [cm ⁻¹] | S_{eff} | μ_{calc} [cm ² V ⁻¹ s ⁻¹] | μ_{FET} [cm ² V ⁻¹ s ⁻¹] |
|----------|---------------------------------------|-----------|--------------------------------------------------------------------|-------------------------------------------------------------------|
| Hole | 968 | 2.19 | 1.15 x10 ⁻¹ | 1.5x10 ⁻⁴ |
| Electron | 978 | 2.26 | 1.82 x10 ⁻¹ | 2.4x10 ⁻¹ |

Table S3. Charge transport data for molecule C3-NT4N: effective frequency ω_{eff} and associated HR factor S_{eff} , computed bulk mobility μ_{calc} and experimental FET mobility μ_{FET} .

1.9 Brightness measurements for compound C6-NT4N

Brightness measurements have been done for the devices reported in Fig. 8c giving values of about 20 cd/m² (Fig. S10). We performed the brightness measurements using the standard OLED procedure, so that by keeping the light source far from the detector, in order to satisfy the point-source requirement at the basis of the brightness physical definition. In particular, the sample was kept at 10 and 20 cm far from the detector. Considering that the highest dimension of emitting OLET area is 1,2 cm, and that the detector surface is 1 cm x 1cm, the point source approximation can be considered satisfied. Moreover, at these distances the detector surface can be approximated with a portion of a sphere surface, so delimiting the solid angle portion used to calculate the brightness value.

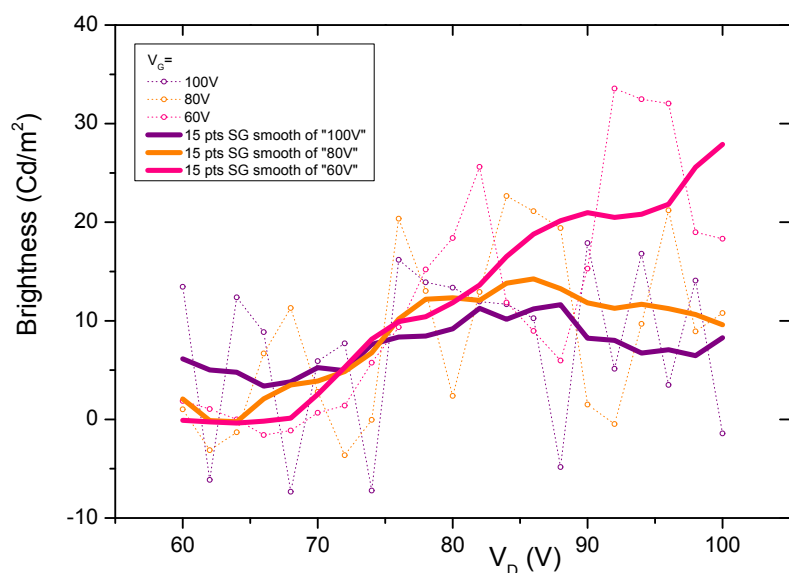


Figure S10. Brightness vs drain voltage for compound C6-NT4N at three different gate voltages.

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