Synthesis of low band gap polymers based on bisthiazole and thienylenevinylene for organic thin-film transistors (OTFTs)

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Figure S1. DSC curves of polymers P1-P4.
Figure S2. Surface morphology images of as cast film of polymer P1 (a), P2 (b), P3 (c), and P4 (d) in bottom-gate top-contact configuration.

Figure S3. X-ray diffraction spectra of as cast film of polymer P1 (a), P2 (b), P3 (c), and P4 (d) at annealing temperature 150 °C.
The X-ray crystal structure of 2b

The crystal structure of 2b (Figure S3) shows the PBTz core to be essential flat, the eleven atoms of the C₆N₃S₂ unit being coplanar to within ca. 0.02 Å.

Crystal data for 2b: C₄₀H₇₅N₃S₂Si₂, M = 718.33, triclinic, P-1 (no. 2), a = 7.6455(3), b = 11.9092(3), c = 25.1027(6) Å, α = 83.133(2), β = 82.326(2), γ = 74.997(3)°, V = 2179.31(12) Å³, Z = 2, Dₐ = 1.095 g cm⁻³, μ(Mo-Kα) = 0.206 mm⁻¹, T = 173 K, colourless tabular needles, Oxford Diffraction Xcalibur 3 diffractometer; 14167 independent measured reflections (R(int) = 0.0521), F² refinement,[x₁] R₁(obs) = 0.0794, wR₂(all) = 0.1774, 9601 independent observed absorption-corrected reflections [|F₀| > 4σ(|F₀|), 2θ_max = 66°], 437 parameters. CCDC 1512672.

Figure S3. The crystal structure of 2b. (50% probability ellipsoids).

TDDFT Calculations

Excited State 1: Singlet-A  2.0835 eV  595.09 nm  f=8.3884  <S**2>=0.000
   422 -> 431      -0.10077
   423 -> 430      -0.13602
   424 -> 429      -0.19610
Excited State 2: Singlet-A 2.2720 eV 545.70 nm f=0.0001 <S**2>=0.000

Excited State 3: Singlet-A 2.5066 eV 494.64 nm f=0.7707 <S**2>=0.000

References

[X1] (a) SHELXTL, Bruker AXS, Madison, WI; (b) SHELX-97, G.M. Sheldrick, Acta Cryst., 2008, A64, 112-122; (c) SHELX-2013, G.M. Sheldrick, Acta Cryst., 2015, C71, 3-8.