

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

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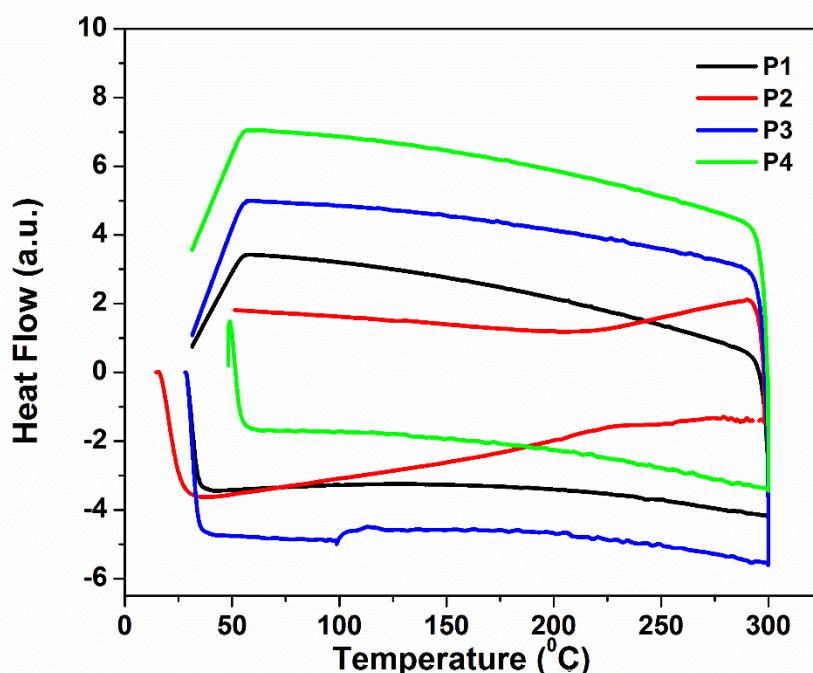
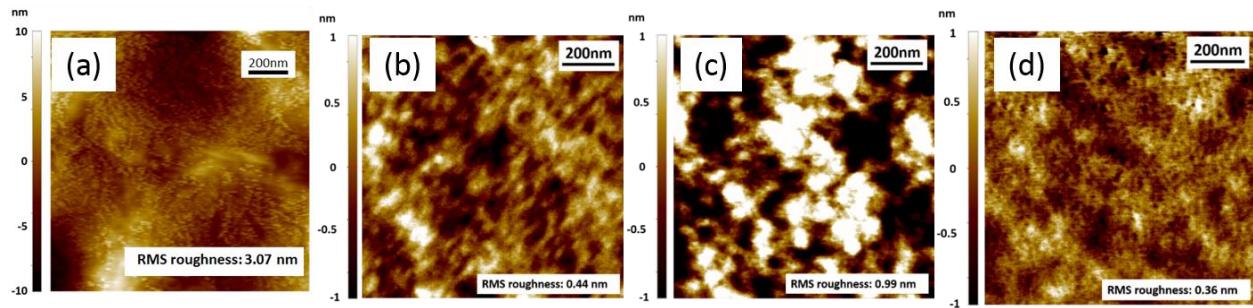
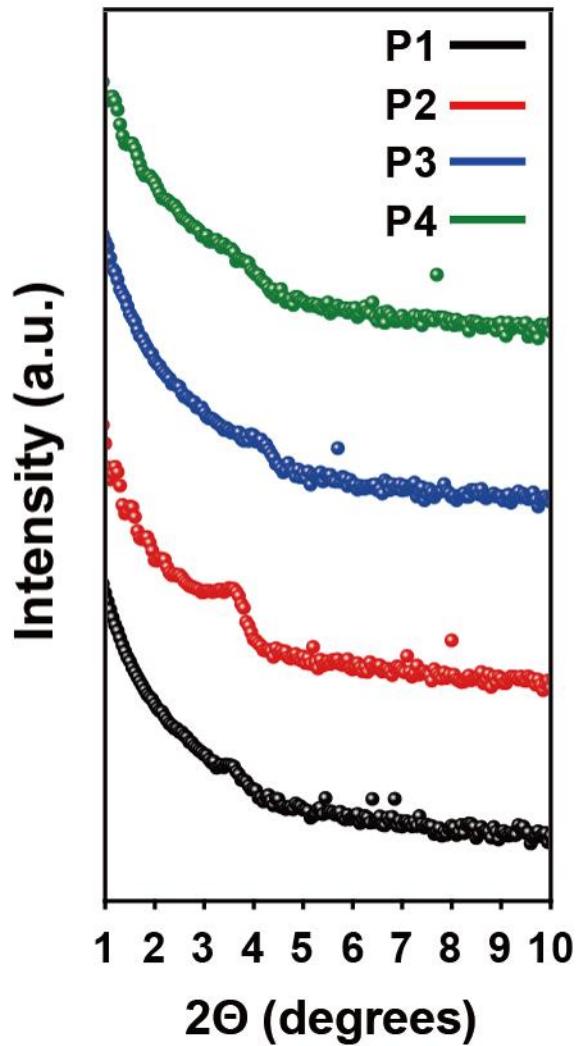


Figure S1. DSC curves of polymers P1-P4.



**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.

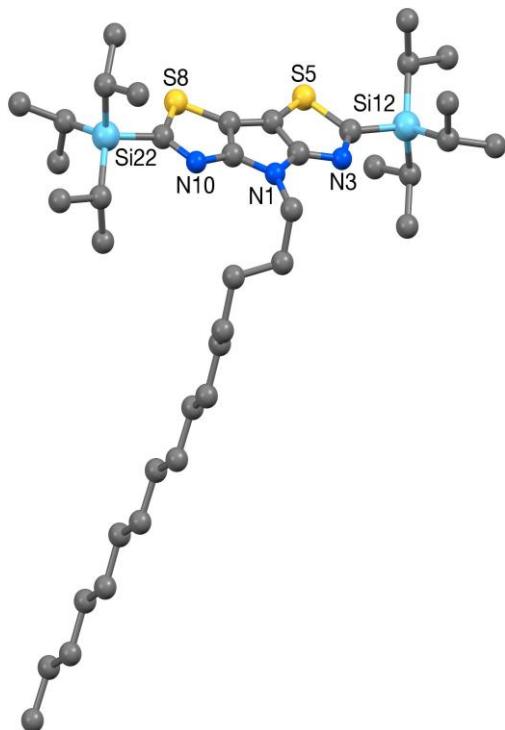


**Figure S3.** X-ray diffraction spectra of as cast film of polymer **P1** (a), **P2** (b), **P3** (c), and **P4** (d) at annealing temperature 150 °C.

## The X-ray crystal structure of **2b**

The crystal structure of **2b** (Figure S3) shows the PBTz core to be essentially flat, the eleven atoms of the C<sub>6</sub>N<sub>3</sub>S<sub>2</sub> unit being coplanar to within ca. 0.02 Å.

*Crystal data for **2b**:* C<sub>40</sub>H<sub>75</sub>N<sub>3</sub>S<sub>2</sub>Si<sub>2</sub>,  $M = 718.33$ , triclinic,  $P\bar{1}$  (no. 2),  $a = 7.6455(3)$ ,  $b = 11.9092(3)$ ,  $c = 25.1027(6)$  Å,  $\alpha = 83.133(2)$ ,  $\beta = 82.326(2)$ ,  $\gamma = 74.997(3)$ °,  $V = 2179.31(12)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_c = 1.095$  g cm<sup>-3</sup>,  $\mu(\text{Mo-K}\alpha) = 0.206$  mm<sup>-1</sup>,  $T = 173$  K, colourless tabular needles, Oxford Diffraction Xcalibur 3 diffractometer; 14167 independent measured reflections ( $R_{\text{int}} = 0.0521$ ),  $F^2$  refinement,<sup>[X1]</sup>  $R_1(\text{obs}) = 0.0794$ ,  $wR_2(\text{all}) = 0.1774$ , 9601 independent observed absorption-corrected reflections [ $|F_0| > 4\sigma(|F_0|)$ ,  $2\theta_{\text{max}} = 66$ °], 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

425 -> 428 0.29583  
426 -> 427 0.52086

Excited State 2: Singlet-A 2.2720 eV 545.70 nm f=0.0001 <S\*\*2>=0.000  
423 -> 429 0.10726  
424 -> 428 0.16851  
424 -> 430 0.13326  
425 -> 427 0.39337  
425 -> 429 -0.19201  
426 -> 428 0.40857

Excited State 3: Singlet-A 2.5066 eV 494.64 nm f=0.7707 <S\*\*2>=0.000  
423 -> 428 0.13216  
424 -> 427 -0.34248  
424 -> 429 0.10162  
424 -> 431 0.10271  
425 -> 428 -0.31686  
425 -> 430 -0.16635  
426 -> 429 0.36189

## 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.