DESIGN OF SEMICONDUCTING POLYMERS TOWARDS HIGHLY THERMALLY STABLE SOLAR CELLS

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In this contribution, we describe the synthesis, electronic structure, and ordering structure of copolymers consisting of thiophene, thiazolothiazole (TzTz) and naphthobisthiadiazole (NTz) in the backbone (PTzNTzs, **Figure 1**), and the performance and thermal stability of their solar cells. Number average molecular weights of PTzNTzs were 30–50 kDa. PTzNTzs had both narrow band gap (ca. 1.55 eV) (**Figure 2a**) and low-lying HOMO energy level (ca. –5.25 eV) (**Figure 2b**), which can contribute to provide high short-circuit currents (J_{SC}) and high open-circuit voltages (V_{OC}). It was found that PTzNTzs formed face-on orientation, which is suitable for solar cells, with relatively narrow π–π stacking distances of around 3.6 Å.

PTzNTz-EHBO with the shortest alkyl side chains had the highest crystallinity in these polymers. PTzNTz-EHBO-based cells exhibited PCEs as high as 9.0% (J_{SC} = 16.0 mAcm^{-2}, V_{OC} = 0.84 V, FF = 0.67) (**Figure 3a, b**) without using solvent additives. The solar cells using other polymers fabricated without a solvent additive, 1,8-diiodooctane (DIO), showed low PCEs of around 1-2%, those with DIO showed significantly enhanced PCEs of up to 8.8%.[1]

Interestingly, the PTzNTzs cells demonstrated excellent thermal stability as they showed negligible degradation after 1000 hour-storage at 85 °C under N_2 atmosphere (**Figure 4**). To the best of our knowledge, the PTzNTzs cells are one of the best performing polymer solar cells in terms of having high PCE and high stability at the same time. These results indicate that PTzNTzs are promising polymers for practical application.

[1] M. Saito, I. Osaka, Y. Suzuki, K. Takimiya, T. Okabe, S. Ikeda, T. Asano, *Sci. Rep.*, **2015**, 5, 14202.

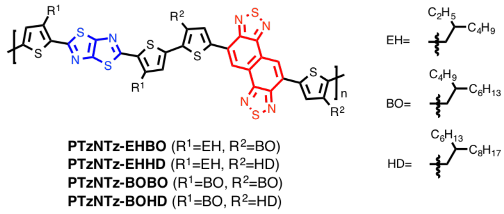

Figure 1 Chemical structure of PTzNTzs.

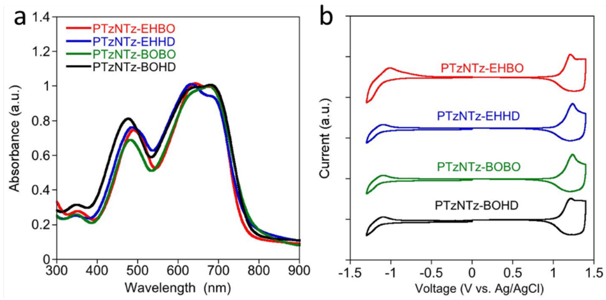

Figure 2 UV-vis absorption spectra of PTzNTzs (a), Cyclic voltrammgram of PTzNTzs (b).

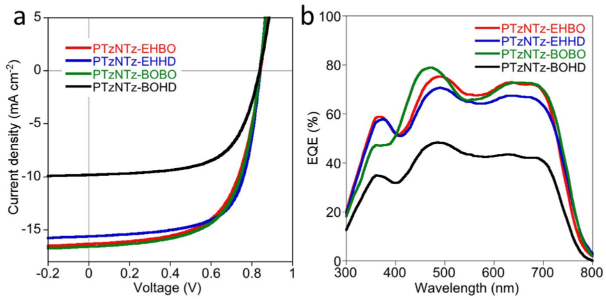

Figure 3 *J-V* curve (a) and EQE spectra (b) of PTzNTz cells.

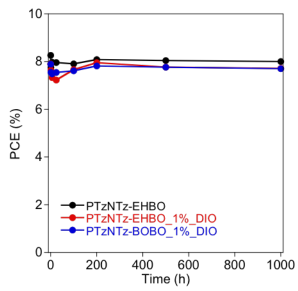

Figure 4 Change of PCE for the cells using PTzNTzs under the storage for 1000 hours at 85°C in the glovebox.