Supporting Information

Optimizing the Thermoelectric Performance of Conjugated Polymer Backbones via Incorporating Tailored Platinum (II) Acetylides

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1. Instrumentation

^{1}H NMR spectra was obtained through Bruker AVANCE Ⅲ 500 MHZ NMR spectrometer in 1,2-dichlorobenzene-d_4, with the internal standard of tetramethylsilane. The molecular weight and distribution of the polymers were measured by PL-GPC220 using polystyrene as calibration standard and 1,2,4-trichlorobenzene as eluent (1.0 mL/min) at 150℃. Thermogravimetric analysis (TGA) was tested on TGA-Q55 system (New Castle, DE, USA) with a heating rate of 10 ^{o}C/min. Fourier transform infrared (FTIR) spectra of these polymers were received from FTIR spectrometer (Nicolet 6700, Thermo Fisher Scientific, Waltham, MA, USA). The UV-vis-NIR absorption spectra in dilute chlorobenzene solutions were

investigated from Lambda 950 spectrophotometer (PerkinElmer, Waltham, MA, USA). Scanning electron microscope (SEM) images of the polymer surfaces before and after doped with $FeCl_3$ were obtained by SEM (SU-70, Tokyo, Japan). The electrochemical properties of materials were collected by CHI 660E electrochemical workstation (Chenhua Instruments Co., Shanghai, China). The X-ray photoelectron spectroscopy (XPS) of the investigated samples were determined by XPS spectroscopy (ESCALAB 250Xi, Thermo Fisher Scientific, Waltham, MA, USA).

2. Energy dispersive spectrometer measurements.

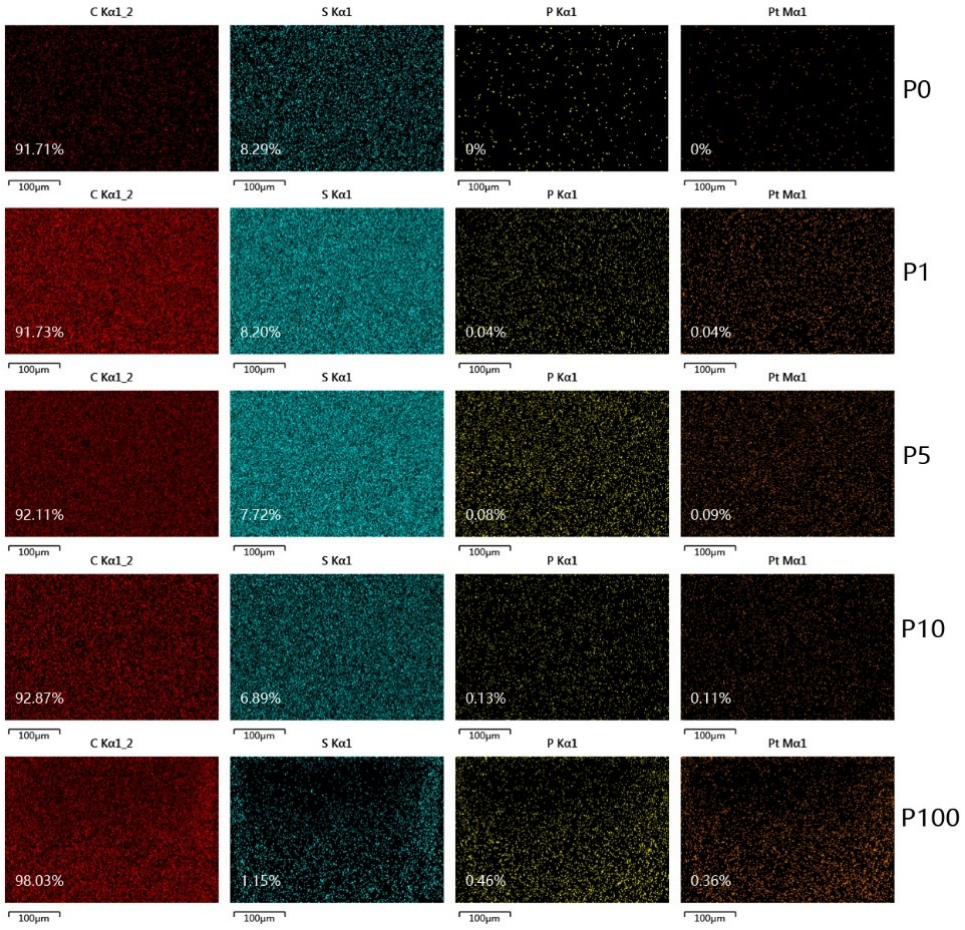


Figure S1 The energy dispersive spectrometer images of P0-P100.

3. FT-IR measurements.

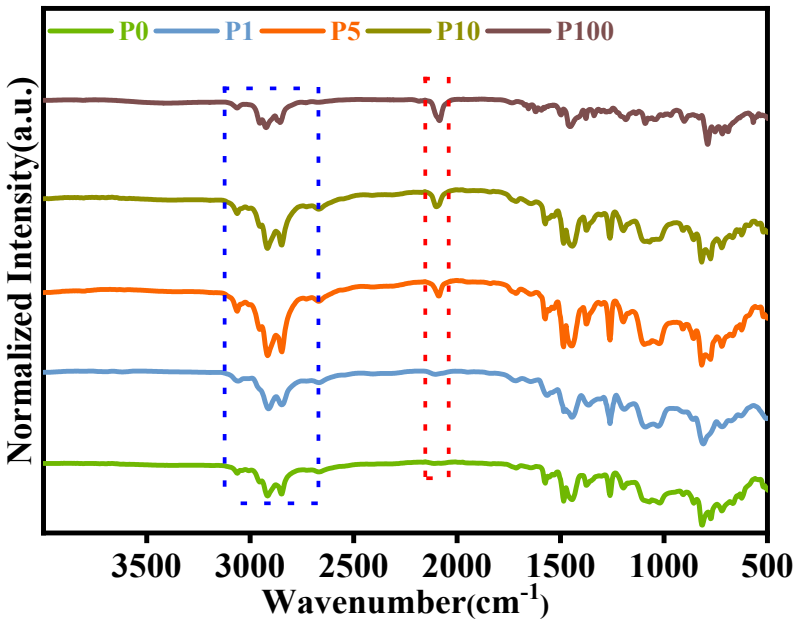


Figure S2. FT-IR absorption spectra of P0-P100.

4. Thermal stabilities.

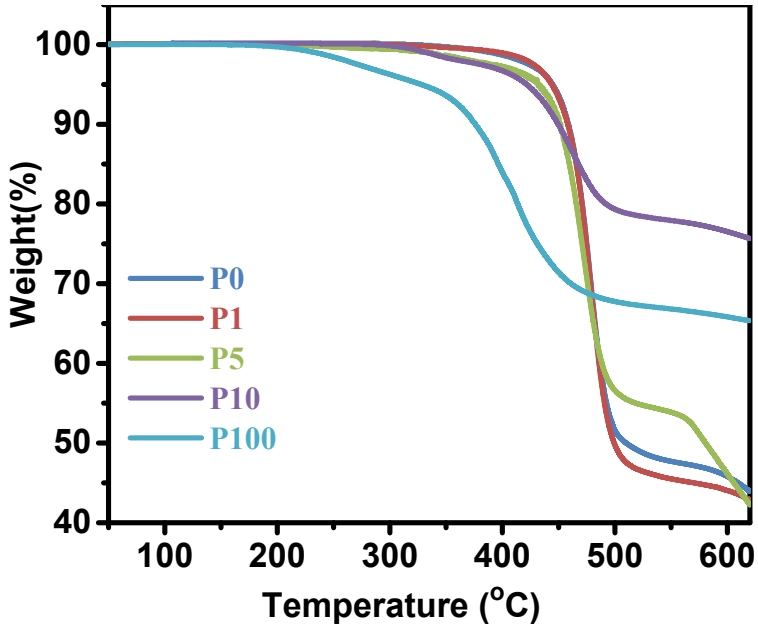
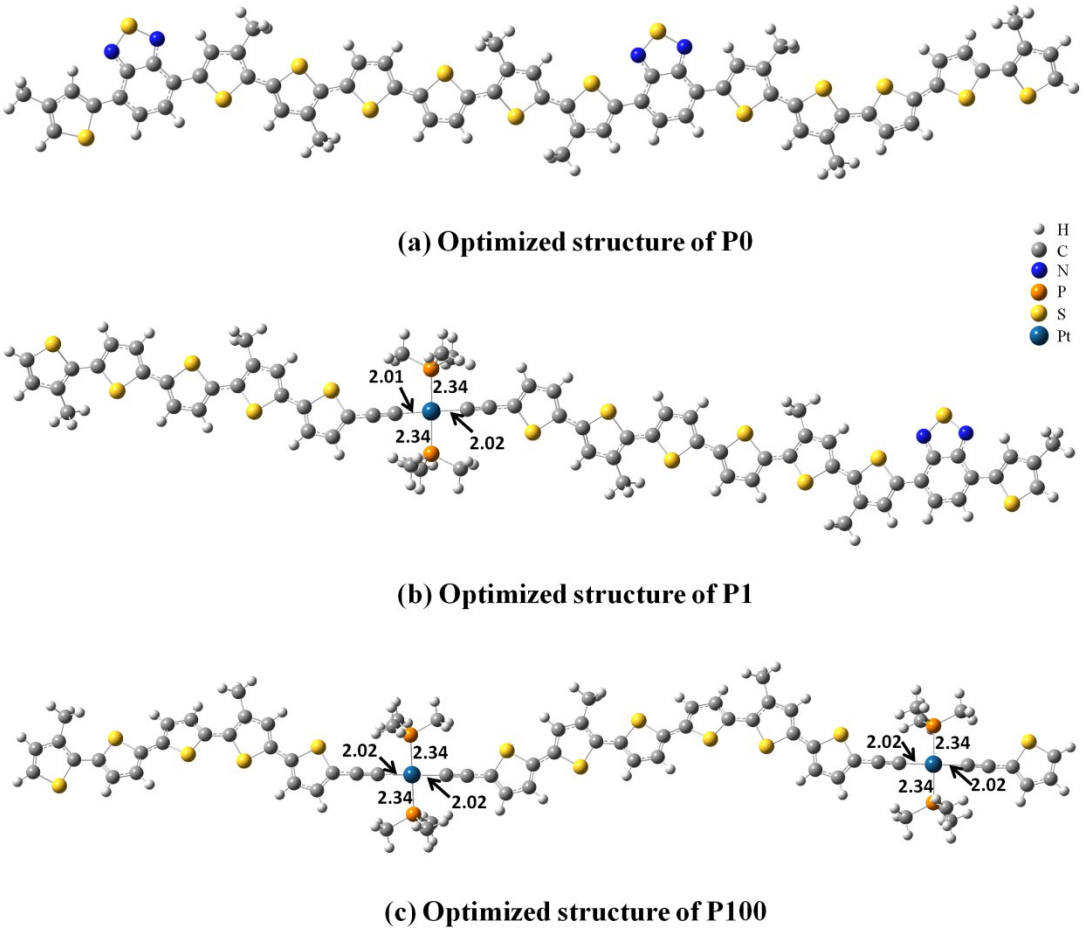


Figure S3. Thermal gravimetric analysis (TGA) curves of the P1-P100.

5. Density functional theory simulations.



(a) Optimized structure of P0

(b) Optimized structure of P1

(c) Optimized structure of P100

Figure S4. Optimized molecular structures of a) P0, b) P1 and c) P100. To simplify the calculations, the dimer model with the alkyl chain replaced with methyl group was carried out.