

Combined nanoarchitectonics with self-assembly and electrosynthesis for flexible PTCDI@PEDOT films with interpenetrating P-N heterojunction

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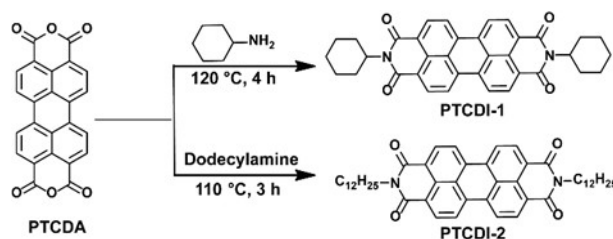
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1. Synthesis of PTCDIs

Two PTCDIs (Scheme S1) were synthesized following our previous work.¹ N,N'-di(cyclohexyl)-3,4,9,10-perylene tetracarboxylic diimide (PTCDI-1): PTCDA (0.20 g, 0.51 mmol), cyclohexylamine (0.50 mL, 4 mmol), and imidazole (5 g) were stirred and heated during 4 h at 120 °C under a N₂ atmosphere. The reaction mixture was then cooled to 25 °C and dispersed in ethanol (30 mL) followed by the addition of 2 M HCl (20 mL) and distilled water (30 mL). The mixture was then stirred overnight. It was washed thoroughly with distilled water until the pH of washings became neutral. The collected solid was vacuum dried at 60 °C. N,N'-di(dodecyl)-3,4,9,10-perylene tetracarboxylic diimide (PTCDI-2): PTCDA (1.42 g, 3.60 mmol) and dodecylamine (2.78 g, 15 mmol) were combined along with anhydrous zinc acetate (25 mg, 0.11 mmol) in imidazole (5 g). The reaction system was heated under N₂ at 110 °C. After the reaction continued for 3 h, the reaction was cooled to 60 °C and dispersed in ethanol (100 mL) followed by the addition of 2 M HCl (300 mL). The mixture was stirred for 12 h. The combined mixture was washed with water (200 mL) and methanol (100 mL). The resulting dark red solid was dried at 60 °C.



Scheme S1 Syntheses of PTCDIs.

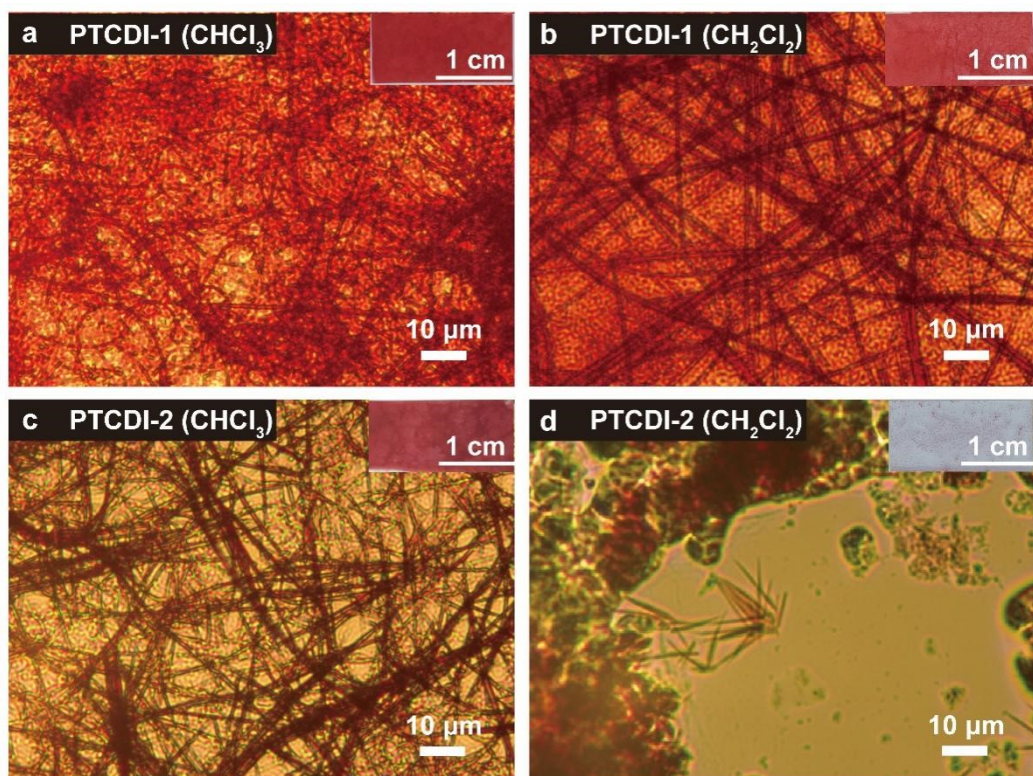


Figure S1. Optical microscope images of PTCDIs nanofibers. The insets are photos of PTCDIs nanofiber electrodes.

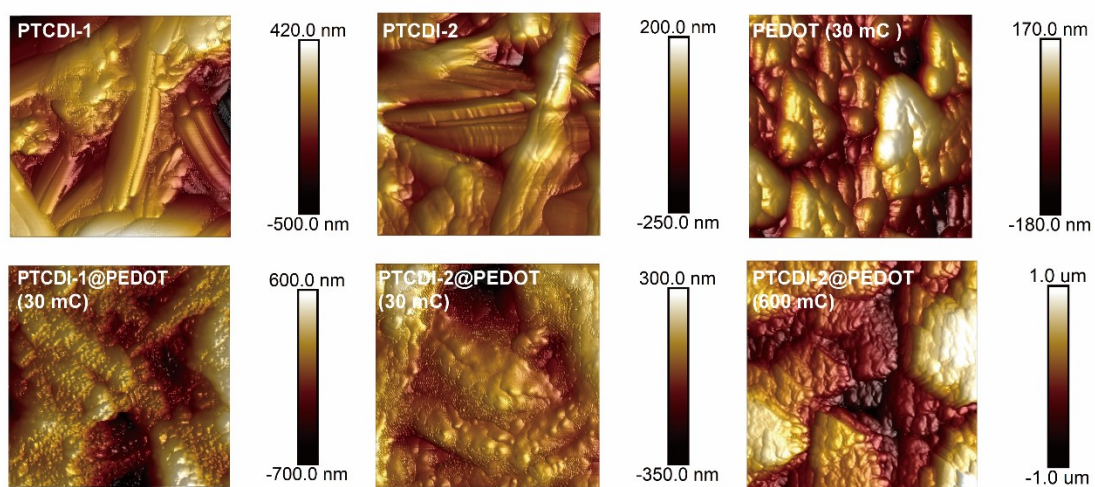


Figure S2. AFM images of PTCDIs nanofibers, PEDOT film and PTCDIs@PEDOT films.

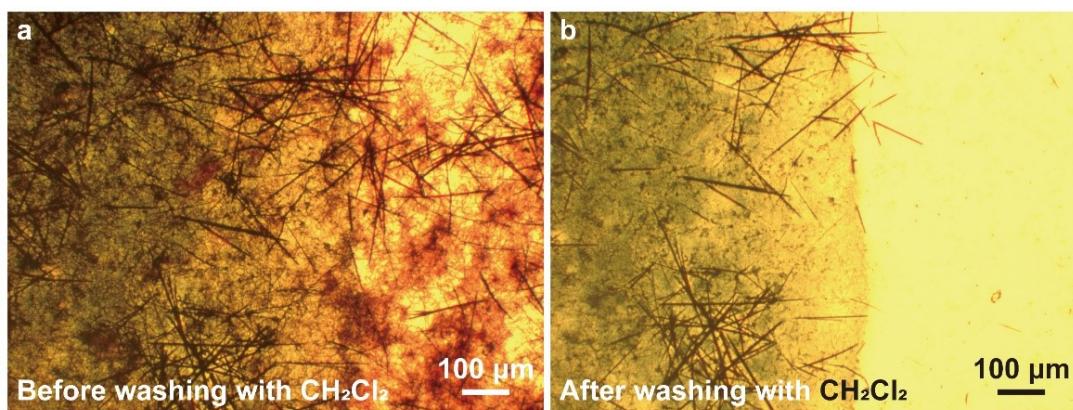


Figure S3. Optical microscope images of PTCDI-1/PEDOT (100 mC) (a) before and (b) after CH₂Cl₂ washing. Area containing PEDOT retained PTCDI-1 nanofibers after washing by CH₂Cl₂.

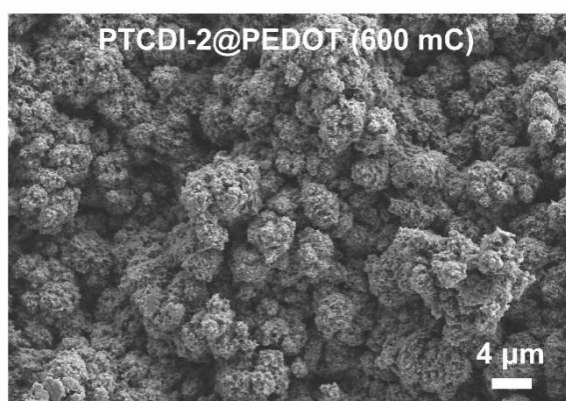


Figure S4. SEM images of PTCDI-2@PEDOT (600 mC) film.

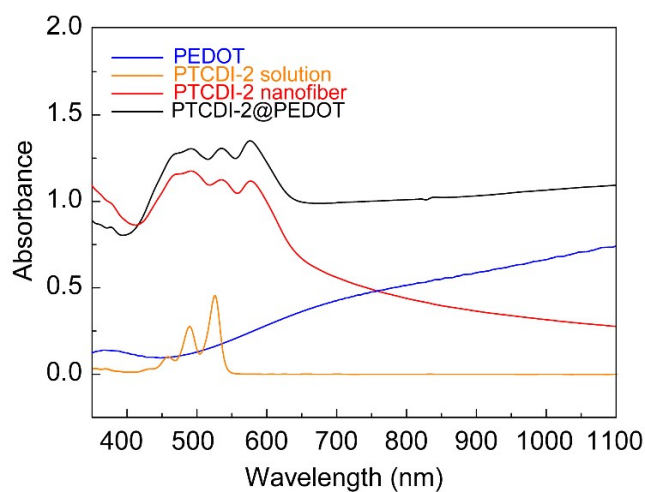


Figure S5. UV-vis spectra of PEDOT film (synthesized under polymerization charge of 30 mC), 5 μM CHCl₃ solution of PTCDI-2, film of PTCDI-2 nanofibers deposited on ITO glass, and film of PTCDI-2@PEDOT (30 mC).

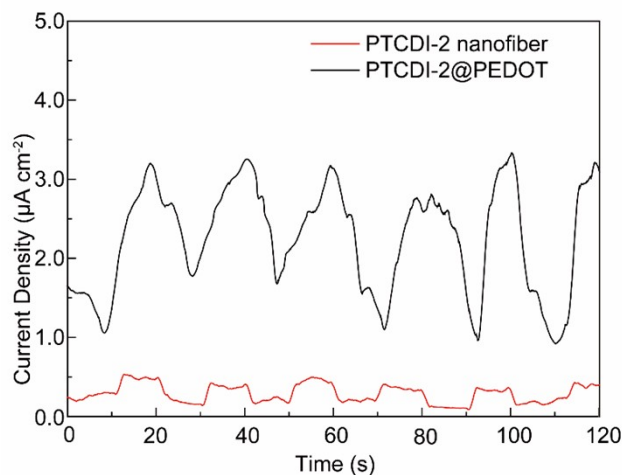


Figure S6. Photocurrent measured for PTCDI-2@PEDOT nanofiber composite film in comparison to pure PTCDI nanofiber film under white light irradiation ($300 \text{ mW} \cdot \text{cm}^{-2}$).

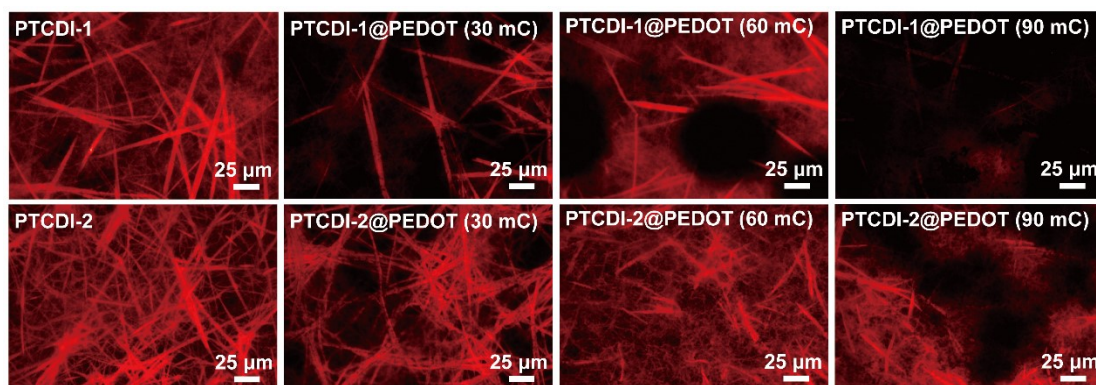


Figure S7. Fluorescence microscope images of PTCDIs nanofiber films and PTCDIs@PEDOT films.

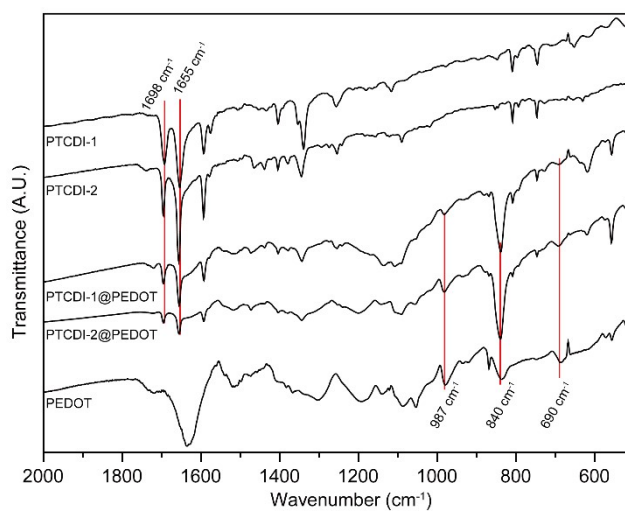


Figure S8. FT-IR spectra of as-prepared samples, PTCDI-1, PTCDI-2, PTCDI-

1@PEDOT, PTCDI-2@PEDOT, and pure PEDOT. The peaks at 1655 cm⁻¹ and 1698 cm⁻¹ are attributed to C=O stretching vibration from amide bond of PTCDis.^{1,2} Typical characteristic peaks for PEDOT can be found at 690, 840 and 987 cm⁻¹ due to the stretching vibrations of C-S-C bond in thiophene ring.³ The result shown here indicates the successful synthesis of the samples..

References:

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- [2] Y. Cheng, R. Q. Song, K. Wu, N. Peng, M. Yang, J. Luo, T. Zou, Y. G. Zuo and Y. Liu, *J. Hazard. Mater.*, 2020, **383**, 121166.
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