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Modulation and Evaluation of Charge Carrier Mobility in Polymer Alloy of Polythiophene and Insulating Matrix with Electron Accepting Molecule

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Experimental

Perylene-3,4,9,10-tetracarboxylic di(10-nonyldecyl)imide (**1**).[S1] Perylenedianhydride (1.34 g, 3.4 mmol), 10-nonyldecylamine[S2] (2.67 g, 8.7 mmol), and imidazole (5.5 g) were heated under N_2 at 120 ˚C for 3 h. To the reaction flask, toluene (10 mL) was added and cooled to room temperature. The product was precipitated into ethanol (100 mL), filtered, washed with methanol, and dried under vacuum. Purification by column chromatography using chloroform as eluent gave a red solid (2.47 g, 78 % yield). ^{1}H NMR ($CDCl_3$): 8.8-8.6 (br, 8H), 5.2 (m, 2H), 2.28 (m, 4H), 1.88 (m, 4H), 1.4-1.2 (br, 56H), 0.84 (t, 12H) ppm.

Perylene-3,4,9,10-tetracarboxylic mon(10-nonyldecyl)imide monoanhydride (**2**). Perylene **1** (2.47 g, 2.7 mmol), potassium hydroxide pellet (85%) (0.37 g, 5.69 mmol), and tert-butyl alcohol (40 mL) were placed in a flask and refluxed at 85 ˚C for 40 min. Acetic acid (40 ml) and HCl_{aq} (15 ml) was added, and the mixture was cooled to room temperature. The product was filtered, and then washed with water to carefully neutralize the product. The crude product was purified by column chromatography with chloroform, to give the desired product as a red solid (1.55 g, 86 % yield). ^{1}H NMR ($CDCl_3$): 8.8-8.6 (br, 8H), 5.2 (m, 1H), 2.28 (m, 2H), 1.88 (m, 2H), 1.4-1.2 (br, 28H), 0.84 (t, 6H) ppm.

Perylene-3,4,9,10-tetracarboxylic mono(10-nonyldecyl)imide mono(6-hydroxyl-hexyl)imide (**3**). Perylene monoanhydride **2** (1.2 g, 1.8 mmol), 6-amino-t-butyldimethylsilylhexan-1-ol (0.84 g, 3.6 mmol),[S3] and imidazole (3.5 g) were heated under N_2 at 125 ˚C for 8 h. To the mixture toluene (10 mL) was added and cooled to room temperature. Methanol (100 mL) was added to quench the reaction. Filtration of the precipitate gave a dark red powder that was dissolved in a dioxane solution of 4M HCl (12.5 mL) and stirred at 30 ˚C for 24 h. This mixture was precipitated into methanol (200 mL). The precipitate was filtered and dried in a vacuum oven to give the crude product, which was further purified by column chromatography (methanol-chloroform mixtures) to give the pure product as a red powder (1.1 g, 80 % yield). ^{1}H NMR ($CDCl_3$): 8.7-8.3 (br, 8H), 5.20 (m, 1H), 4.18 (t, 2H), 3.70 (t, 2H), 2.30 (m, 2H), 1.94 (m, 2H), 1.87 (m, 2H), 1.66 (m, 2H), 1.50 (m, 4H), 1.4-1.2 (br, 28H), 0.84 (t, 6H) ppm.

Perylene-3,4,9,10-tetracarboxylic mono(10-nonyldecyl)imide mono(6-hexyl acrylate) imide (**4**). To a solution of perylene 3 (1.34 g, 1.7 mmol) in anhydrous methylene chloride (20 mL)

was added acryloyl chloride (3.6 mL, 43.7 mmol). The mixture was stirred for 24 h, and then precipitated into methanol (150 mL). The precipitate was filtered and dried under vacuum. The crude product was purified column chromatography (chloroform-methanol mixtures) to give the desired product as a red powder (1.1 g, 81 % yield). ^{1}H NMR ($CDCl_3$): 8.7-8.4 (br, 8H), 6.43 (d, 1H), 6.14 (dd, 1H), 5.80 (d, 1H), 5.22 (m, 1H), 4.20 (m, 4H), 2.27 (m, 2H), 1.92 (m, 2H), 1.75 (m, 4H), 1.52 (br, 4H), 1.4-1.2 (br, 28H), 0.85 (t, 6H) ppm.

REFERENCES

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S2) L. D. Wescott, D. L. Mattern, *J. Org. Chem.* **2003**, *68*, 10058.

S3) R. T. Pon, *Tetrahed. Lett.* **1991**, *32*, 1715.

Supporting Figures.

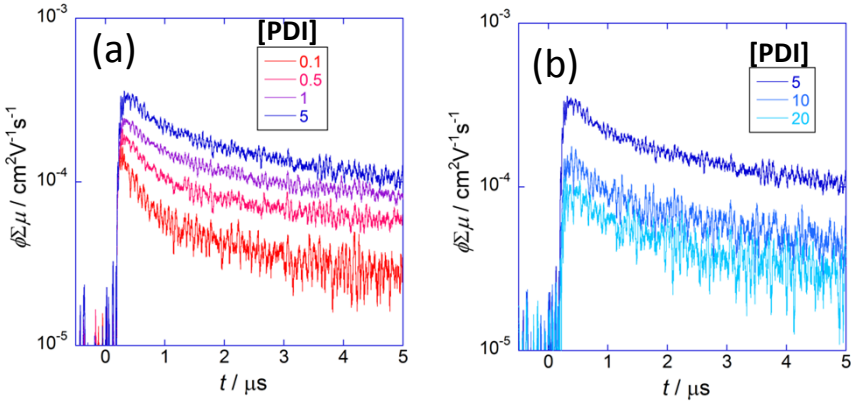

Figure S1. Kinetic decays of simple ternary blends of PS (PMMA) : P3HT : PDI = 100 : 1 : 0.1–20 measured by FP-TRMC (λ_{ex} =355 nm).

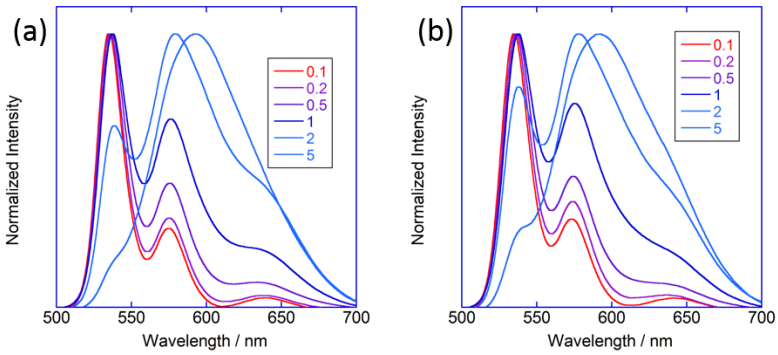

Figure S2. Normalized fluorescence spectra (λ_{ex} = 355 nm) observed in PDI dispersed in (a) PS+P3HT and (b) PMMA+P3HT blend films. Matrix : P3HT : PDI = 100 : 1 : 0.1–5.