

Electronic Supplementary Information for

Alkylsilane functionalized perylenediimide derivatives with
differential gas sensing properties

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1. Synthesis of DMB, TMSA, TESA and TPSA

***N,N'*-bis(*n*-hexadecyl)-1,7-di(3,3-dimethyl-1-butynyl)perylene-3,4,9,10-tetracarboxyl diimide (DMB).** *N, N'*-bis(*n*-hexadecyl)-1,7-dibromoperylene-3,4,9,10-tetracarboxyldiimide (0.12 g, 0.13 mmol), 3,3-Dimethyl-butyne(0.70 g, 0.86 mmol), [Pd(PPh₃)₄] (0.02 g, 0.02 mmol) and CuI were stirred in a mixture of 15 mL of triethylamine and 15 mL of THF for 14 h at 53 °C under argon atmosphere. The mixture was cooled to room temperature and diluted with CH₂Cl₂. The organic layer was washed three times with water to neutral, dried with Na₂SO₄, and the solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel(petroleum ether/CH₂Cl₂,1:1) to yield the red product 0.11 g (86%). ¹H NMR (CDCl₃, 400 MHz) δ(ppm): 0.85~0.89 (m,6 H),1.24~1.25 (m,70 H),1.57~1.58 (m, 4 H), 4.20~4.23 (m,4 H), 8.64~8.66(d, *J* = 8.0, 2 H), 8.76 (s, 2 H),10.12~10.14 (d, *J* = 8.0, 2 H), MS (MALDI-TOF): calcd for C₆₈H₉₀N₂O₄, 999.45 m/z, found 999.32. Anal. Calcd for C₆₈H₉₀N₂O₄ : C, 81.72; H, 9.08; N, 2.80. Found: C, 81.56; H, 8.96; N, 2.91.

***N, N'*-bis(*n*-hexadecyl)-1,7-di(trimethylsilylethynyl)perylene-3,4,9,10-tetracarboxyldiimide (TMSA).** *N, N'*-bis(*n*-hexadecyl)-1,7-dibromoperylene-3,4,9,10-tetracarboxyldiimide (0.14 g, 0.14 mmol), trimethylsilylacetylene (0.08 g, 0.84 mmol), [Pd(PPh₃)₄](0.02 mg, 0.02 mmol) and CuI were stirred in a mixture of 15 mL of triethylamine and 15 mL of THF for 14 h at 53 °C under argon atmosphere. The mixture was cooled to room temperature and diluted with CH₂Cl₂. The organic layer was washed three times with water to neutral, dried with Na₂SO₄, and the solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel(petroleum ether/CH₂Cl₂, 1:1) to yield the red product 0.13 g (88%).¹H NMR (CDCl₃,400 MHz) δ(ppm): 0.85~0.89 (m, 6 H), 1.24~1.42 (m, 70 H),1.72~1.80 (m, 4 H),4.18~4.22 (m, 4 H), 8.57~8.59 (d, *J* = 8.0, 2 H),8.76 (s, 2 H), 10.12~10.14 (d, *J* = 8.0, 2 H), calcd for C₆₆H₉₀N₂O₄ Si₂, 1031.60 m/z, found 1031.33. Anal. Calcd for C₆₆H₉₀N₂O₄ Si₂: C, 76.84; H, 8.79; N, 2.72. Found: C, 76.55; H, 8.92; N, 2.75.

***N,N'*-bis(*n*-hexadecyl)-1,7-di(triethylsilylethynyl)perylene-3,4,9,10-tetracarboxyldiimide (TESA).** *N, N'*-bis(*n*-hexadecyl)-1,7-dibromoperylene-3,4,9,10-tetracarboxyldiimide(0.09 g, 0.1 mmol), (triethylsilyl)acetylene (0.08 g, 0.59 mmol), [Pd(PPh₃)₄] (0.01 g, 0.01 mmol), CuI were stirred in a mixture of 10 mL of triethylamine and 10 mL of THF for 14 h at 53 °C under argon atmosphere. The mixture was cooled to room temperature and diluted with CH₂Cl₂. The organic layer was washed three times with water to neutral, dried with Na₂SO₄, and the solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/CH₂Cl₂,1:1) to yield the red product 0.08 g (76%). ¹H NMR (CDCl₃, 400 MHz) δ(ppm): 0.80~0.83 (m, 24 H),1.13~1.17 (m, 12 H), 1.24~1.28 (m, 52 H),1.72~1.80(m, 4 H), 4.18~4.22 (m, 4 H), 8.52~8.54 (d, *J* = 8.0, 2 H), 8.74 (s, 2 H), 10.17~10.19 (d, *J* = 8.0, 2 H), calcd

for $C_{72}H_{102}N_2O_4 Si_2$, 1115.76 m/z, found 1115.26. Anal. Calcd for $C_{72}H_{102}N_2O_4 Si_2$: C, 77.50; H, 9.21; N, 2.51. Found: C, 77.62; H, 9.18; N, 2.49.

***N,N'*-bis(*n*-hexadecyl)-1,7-di(triisopropylsilylethynyl)perylene-3,4,9,10-tetracarboxydiimide (TPSA).** *N,N'*-bis(*n*-hexadecyl)-1,7-dibromoperylene-3,4,9,10-tetracarboxyl-diimide (0.10 g, 0.10 mmol), (triisopropylsilyl)acetylene (0.09 g, 0.48 mmol), $[Pd(PPh_3)_4]$ (0.01 g, 0.01 mmol), CuI were stirred in a mixture of 10 mL of triethylamine and 10 mL of THF for 14 h at 53 °C under argon atmosphere. The mix was cooled to room temperature and diluted with CH_2Cl_2 . The organic layer was washed three times with water to neutral, dried with Na_2SO_4 , and the solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel(petroleum ether/ CH_2Cl_2 , 1:1) to yield the red product 0.09 g (78%). 1H NMR ($CDCl_3$, 400 MHz) δ (ppm): 1.22~1.28 (m, 94 H), 1.59~1.62 (m, 4 H), 1.75~1.79 (m, 6 H), 4.19~4.23 (m, 4 H), 8.60~8.63 (d, $J = 8.4$, 2 H), 8.82 (s, 2 H), 10.33~10.35 (d, $J = 8.0$, 2 H). calcd for $C_{78}H_{114}N_2O_4 Si_2$, 1199.92 m/z, found 1199.91. Anal. Calcd for $C_{78}H_{114}N_2O_4 Si_2$: C, 78.02; H, 9.58; N, 2.33. Found: C, 78.00; H, 9.65; N, 2.36.

2. Supporting Figures

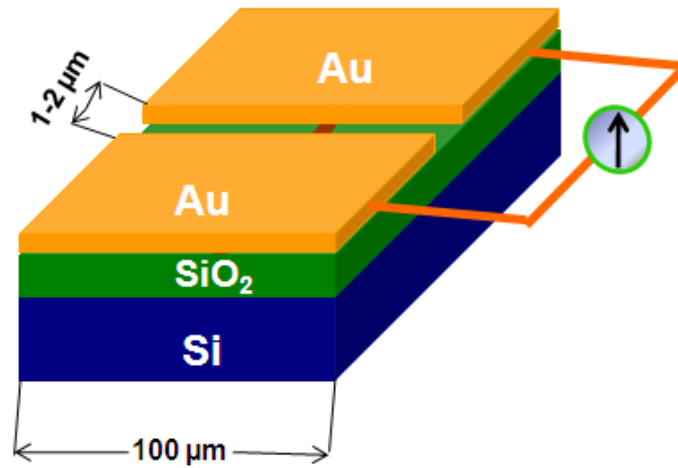


Fig. S1 Schematic image of gas sensing device with length and width of channel.

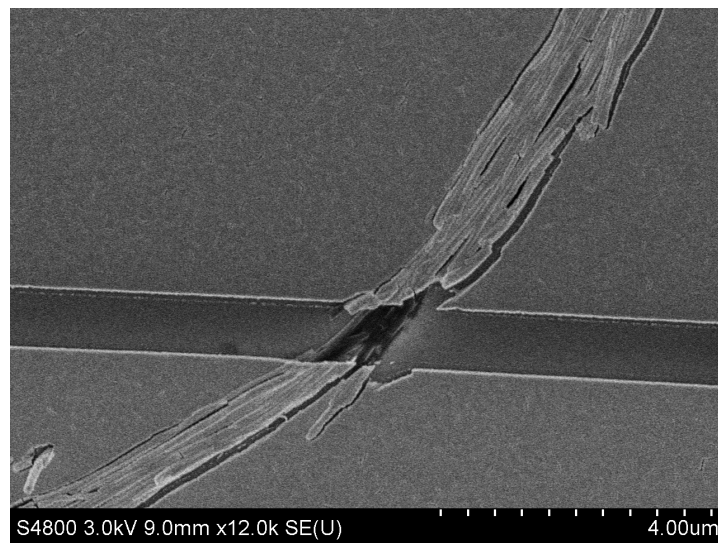


Fig. S2 SEM image of DMB gas sensing device.

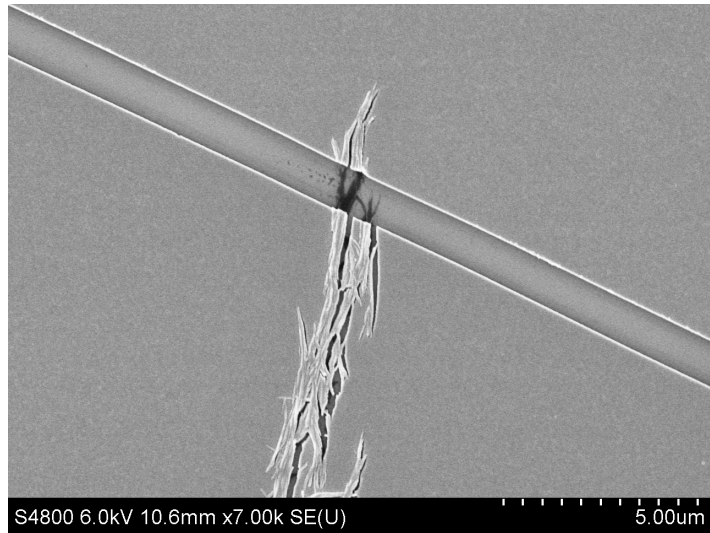


Fig. S3 SEM image of TMSA gas sensing device.

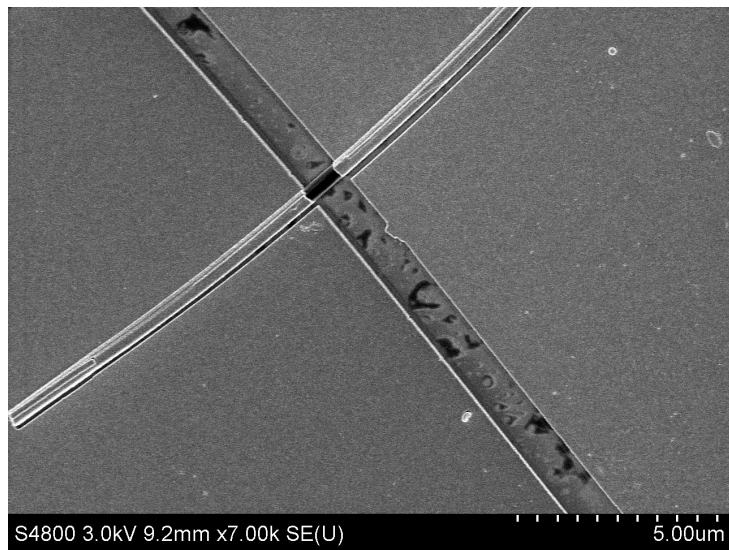


Fig. S4 SEM image of TESA gas sensing device.

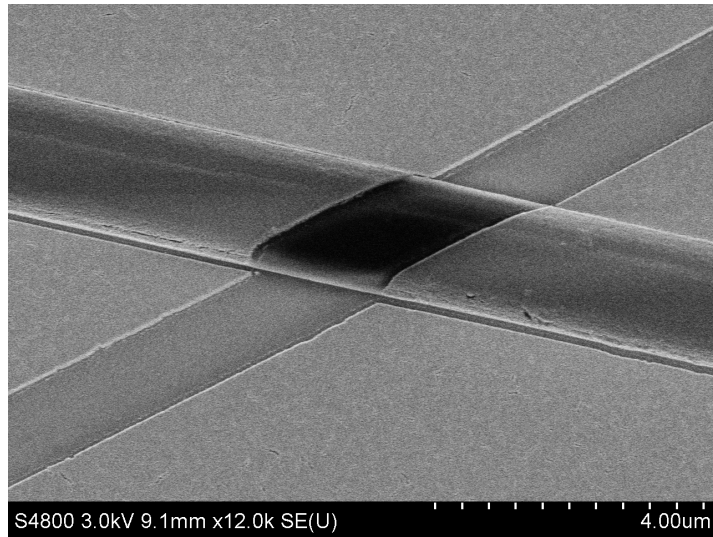


Fig. S5 SEM image of TPSA gas sensing device.