

Supporting Information

Polyurethane Foam Functionalized by AIE-active Polymer using Ultrasonication-assisted Method; Preparation and the Application for detection of explosives.

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General

Dichlorodiphenylsilane, triethylamine (TEA) and 4-hydroxybenzophenone were purchased from Sigma-Aldrich or TCI and used as received without further purification. Other chemicals were used unless otherwise specified. THF was distilled from sodium benzophenone ketyl under dry nitrogen. All the reactions were carried out using Schlenk techniques in nitrogen atmosphere.

The ^1H NMR, ^{13}C NMR and spectra were recorded with a AVANCE III 500 spectrometer. The thermal analyses were performed on Shimadzu DTG-60H thermogravimetric analyzer, in a nitrogen atmosphere at a rate of 10 $^{\circ}\text{C}/\text{min}$. Elementary analysis (EA) was measured on a FLASH EA1112 element analyzer. UV-vis absorption spectra and PL spectra were measured by Shimadzu UV-3100 spectrophotometer and Edinburgh FL/FS920 TCSPC luminescence spectrophotometer, respectively. Molecular weights and polydispersities of the copolymers were determined by gel permeation chromatography (GPC) analysis, with polystyrene standard calibration (waters high-pressure GPC assembly Model M515 pump, 1-Styragel columns of HR4, HR4E, and HR5E with 500 and 100 \AA , refractive index detectors, solvent THF). Cyclic voltammetry (CV) was performed on PARSTAT 2273 system, with a three-electrode cell in a solution of Bu_4NBF_4 (0.1 M) in CH_2Cl_2 , at a scan rate of 100 mV/s. A Pt wire was used as the counter electrode, and an Ag/AgCl (0.1 M) electrode was used as the reference electrode. Prior to each series of measurements, the cell was deoxygenated with nitrogen. The morphologies of modified PU foams were characterized by field emission scanning electron microscopy (FESEM, Hitachi SU70). Fluorescence microscope photos were taken by Zeiss Axio Imager A1.

Caution

PA and DNT are very dangerous, should be store in darkness around 3 $^{\circ}\text{C}$ quietly. When starting examinations, a small amount of the explosives were weighted without any friction or hitting! The PA solution in methanol and DNT powder should also be place in low temperature silently.

Synthesis

TPE-OH was synthesized according to the literature^[1].

PSiTPE To a stirred solution of **TPE-OH** (0.546 g, 1.5 mmol) and **TEA** (0.323 g, 3.2 mmol) in THF (20 mL), dichlorodiphenylsilane (0.403 g, 1.6 mmol) were added. After refluxed for 24 h, phenol was added for end capping. 10 h later, the reaction mixture was extracted with CH_2Cl_2 for 3 times, and dried over MgSO_4 . And then precipitated in methanol, the polymer was obtained as white powder. (80 % yield). ^1H NMR (500 MHz, CDCl_3 , δ): 7.68-7.44 (4H, m), 7.46-7.22 (6H, m), 7.19-7.04 (6H, m), 7.00-6.81 (8H, m), 6.63-6.24 (4H, m). ^{13}C NMR (CDCl_3 , δ): 134.58, 134.97, 134.58, 134.36, 132.86, 132.57, 131.35, 130.39, 127.74, 126.22, 119.22, 114.61. ^{29}Si NMR (CDCl_3 , δ): -121.56. Anal. calcd for $(\text{C}_{38}\text{H}_{28}\text{SiO})_n$: C, 86.36; H, 5.3; found: C, 86.40; H, 5.1.

Reference:

[1] C. Y. K. Chan, J. W. Y. Lam, C. K. W. Jim, H. H. Y. Sung, I. D. William and B. Z. Tang, *Macromolecules*, 2013, 46, 9494.

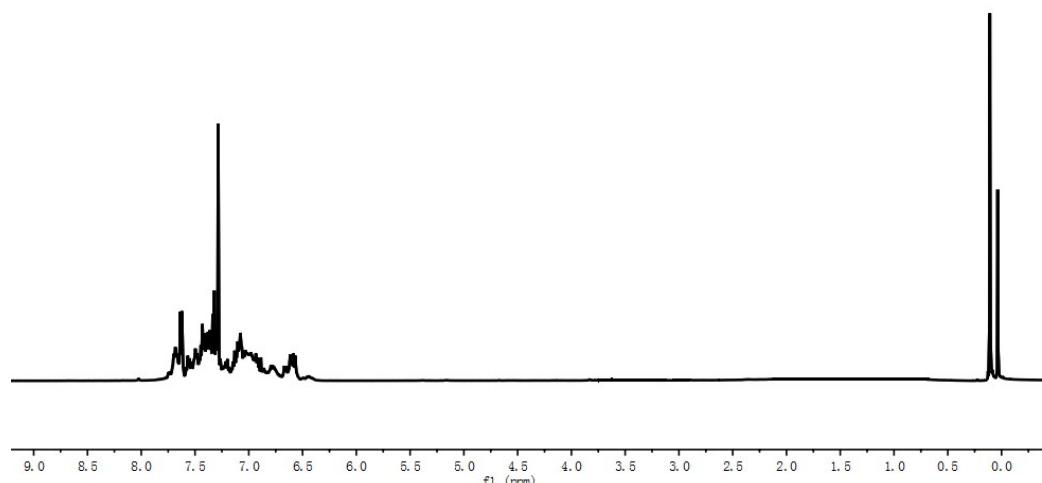


Fig. S1 ^1H NMR spectrum of polymer in CDCl_3

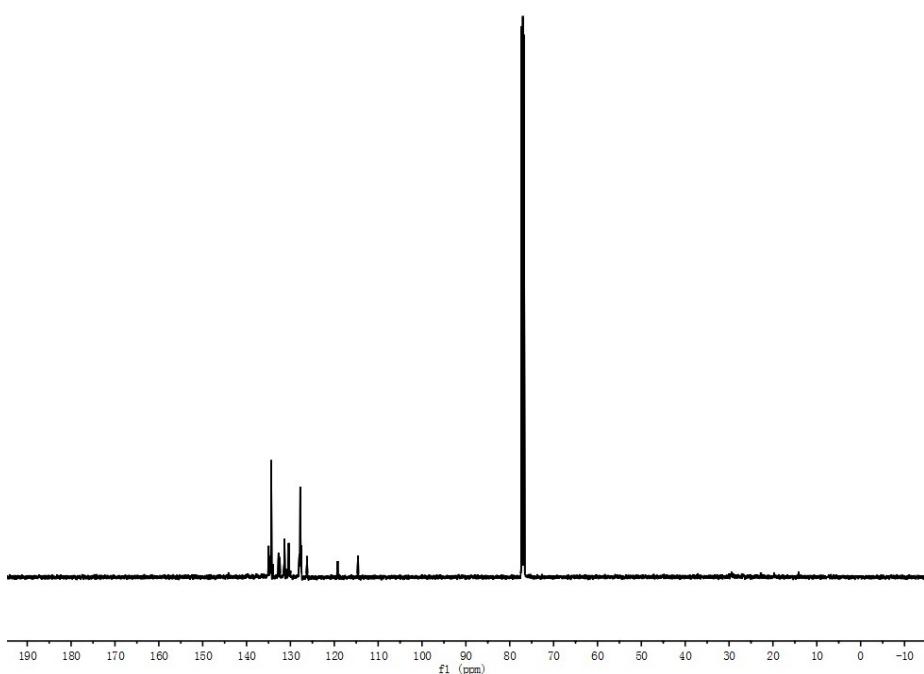


Fig. S2 ^{13}H NMR spectrum of polymer in CDCl_3

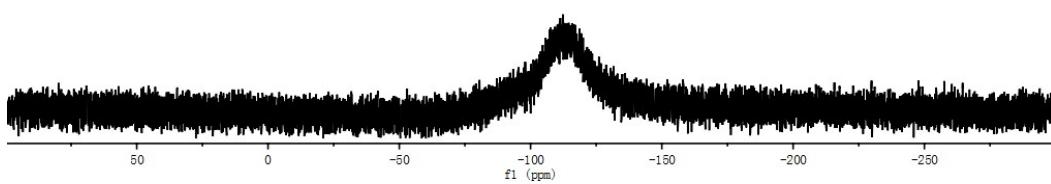


Fig. S3 ^{29}Si NMR spectrum of polymer in CDCl_3

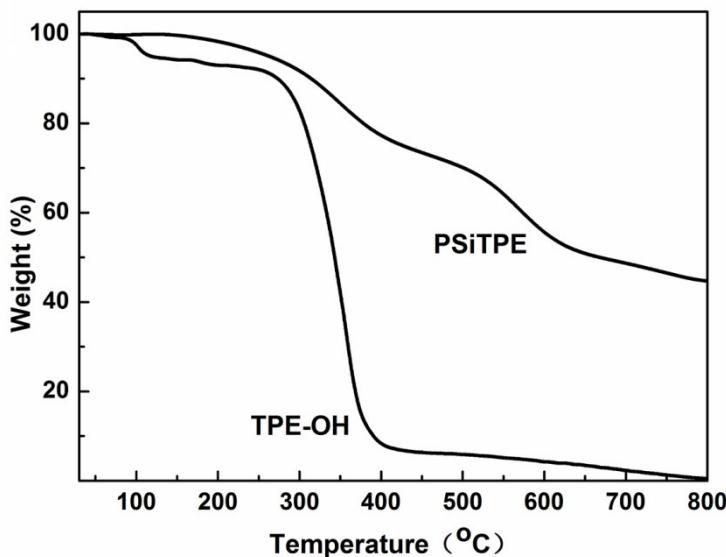


Fig. S4. TGA curves of the polymer and monomer.

Preparation of the decorated PU foams.

The tailored PU foams' model is at the thickness of 2 mm and the radius of 5 mm. Foams washed with water and ethanol were placed in vacuum dry at 60 °C for 24 hours before use.

Part 1. Immersing method: a pill of PU foam was immersed in **PSiTPE** solution (volume, $\text{THF}/\text{H}_2\text{O} = 1/9$, $100 \mu\text{g mL}^{-1}$) for 30 min, and washed with ethanol, dried under vacuum oven at 60 °C for 24 h.

Part 2. Ultrasonication method: Polymer nanoparticles of **PSiTPE** was prepared by vigorously mixing with the concentration of 50, 100, 150 $\mu\text{g mL}^{-1}$ in solution (volume, $\text{THF}/\text{H}_2\text{O} = 1/9$). After that, the nanoparticles were pre-dispersed under ultrasonication for 60 min before anchoring onto the PU foams. Then, PU foam was immersed into the solution and subjected to ultrasonication at a high-intensity ultrasonic for 30 min to obtain the modified PU foam. Finally, the modified PU foam was washed with ethanol for 30 min to remove the unanchored nanoparticles and dried under vacuum oven at 60 °C for 24 h. The as-prepared samples were named PU-50, PU-100 and PU-150.

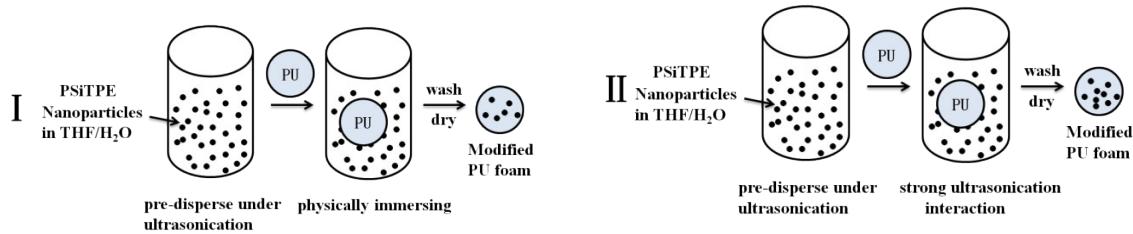


Fig. S5. Schematic diagrams of the two methods: (I) immersing, (II) ultrasonication.

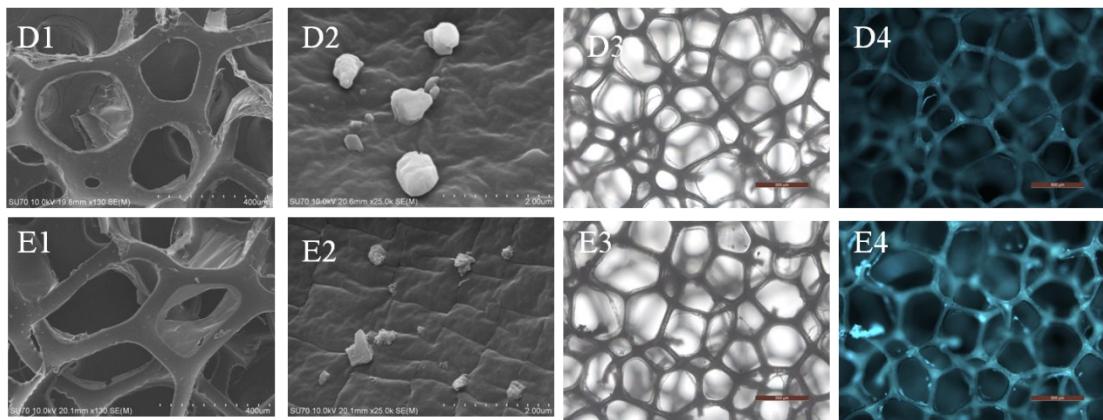


Fig. S6. SEM images and fluorescence microscope photos of PU-50 (D1, D2, D3, D4) and PU-150 (E1, E2, E3, E4).

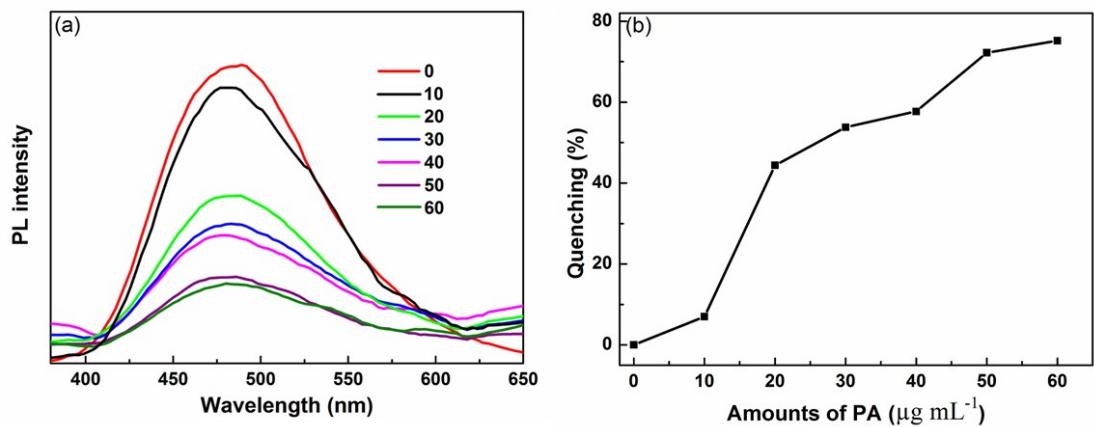


Fig. S7. (a) Fluorescence spectra of PU-50 in the presence of different PA concentrations ($\mu\text{g mL}^{-1}$), (b) Quenching efficiency - PA concentrations curve of PU-50.

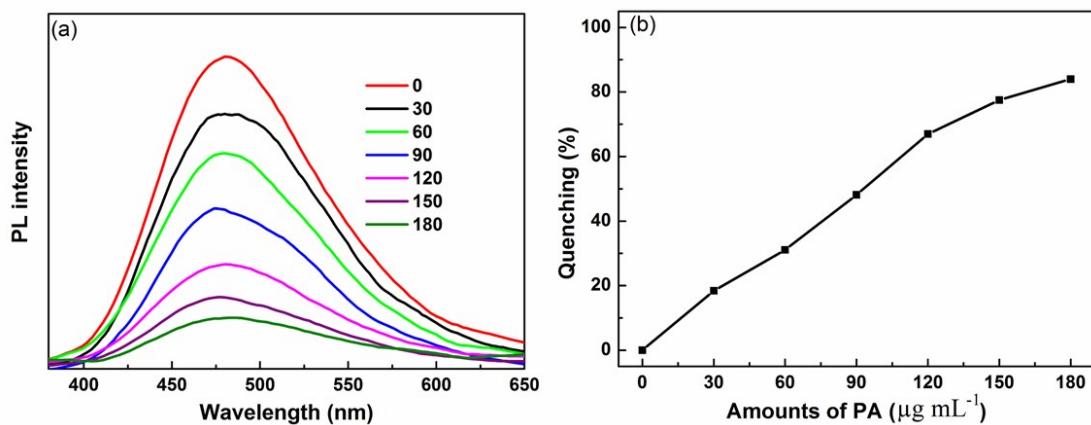


Fig. S8. (a) Fluorescence spectra of PU-150 in the presence of different PA concentrations ($\mu\text{g mL}^{-1}$), (b) Quenching efficiency - PA concentrations curve of PU-150.

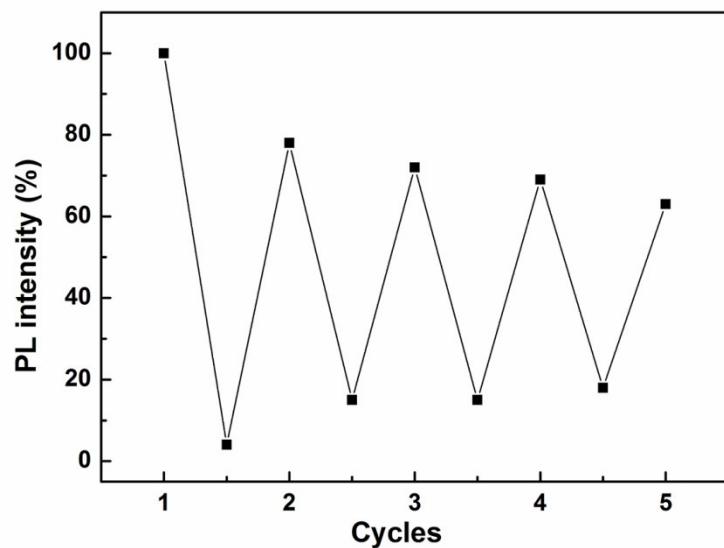


Fig. S9. Fluorescence recovery of PU-2.5 exposing to saturated DNT vapors treated with hydrazine.

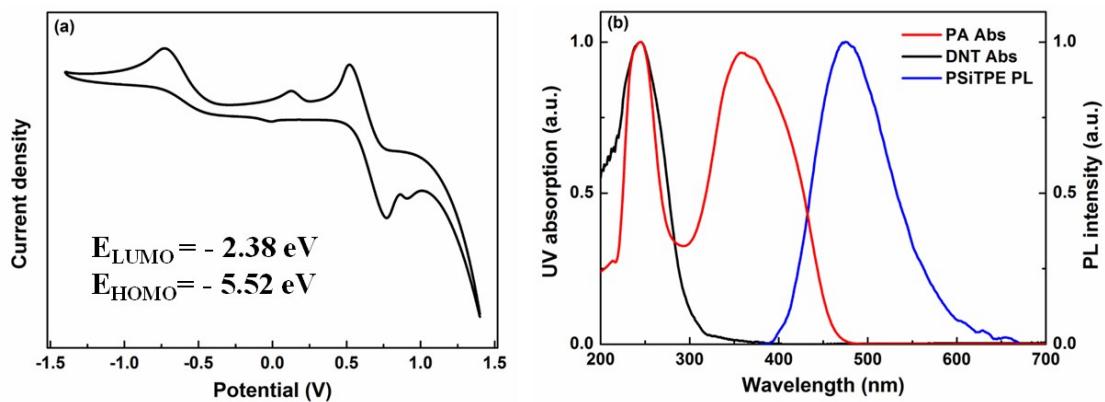


Fig. S10. (a) Cyclic voltammetry curve and the energy levels of **PSiTPE**, (b) Absorption spectrum of PA and DNT, and the emission spectrum of the polymer.