

## Supplemental information

*for*

### Single-layer assembly of pyrene end-capped terthiophene and its sensing performances to nitroaromatic explosives

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### Main Contents

**Figure S1.** The calculated bond lengths and dihedral angles of 3T and the corresponding derivatives at B3LYP/6-311G(d, p) level.

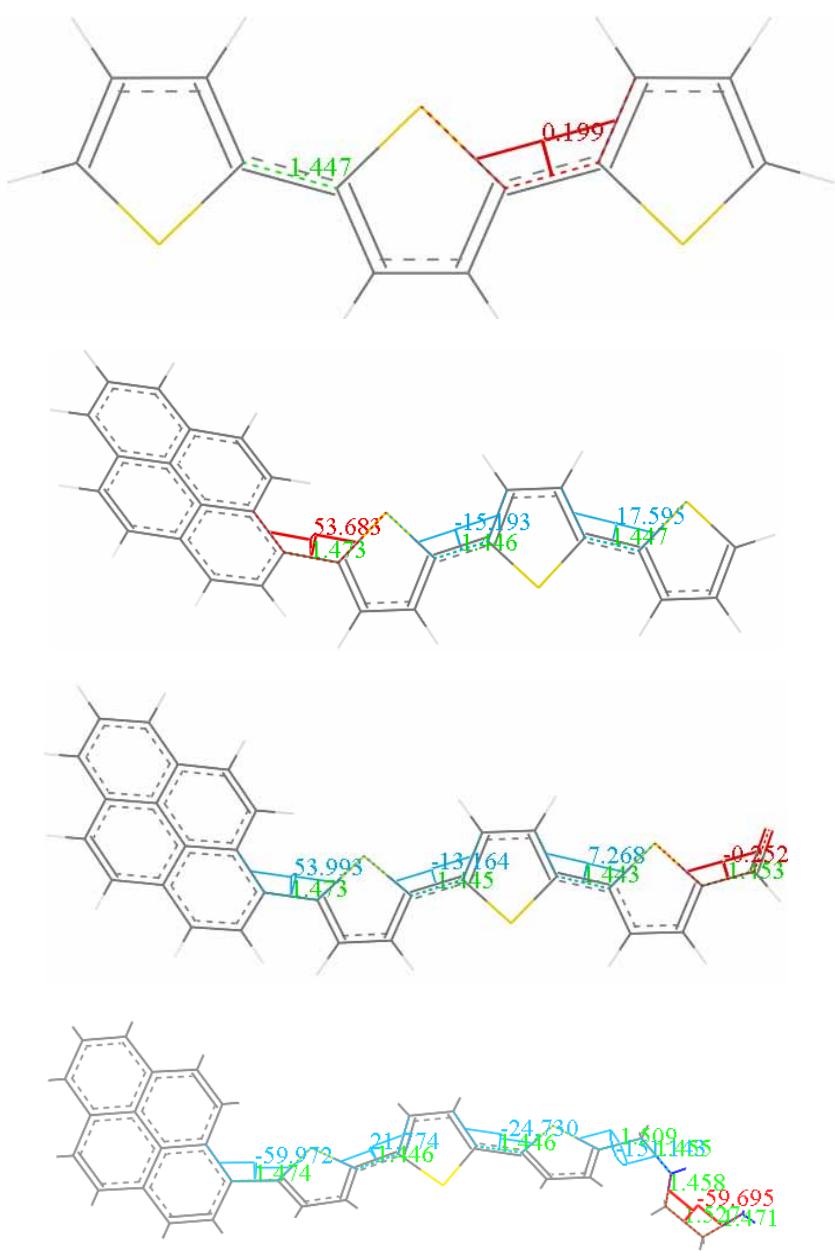
**Figure S2.** Fluorescence excitation ( $\lambda_{\text{Ex}}=396$  nm) and emission ( $\lambda_{\text{Em}}=515$  nm) spectra of PTEA in its  $\text{CH}_2\text{Cl}_2$  solution, the inset display the photos of PTEA under room light (a) and UV light ( $\lambda=365$  nm) illumination (b).

**Figure S3.** Normalized UV-vis absorption spectra of 3T and the corresponding compounds in their  $\text{CH}_2\text{Cl}_2$  solutions and the inset display their calculated optical band gaps (top and middle). Comparison between the calculated excitation energies of the three compounds and those determined via UV-vis measurements (bottom).

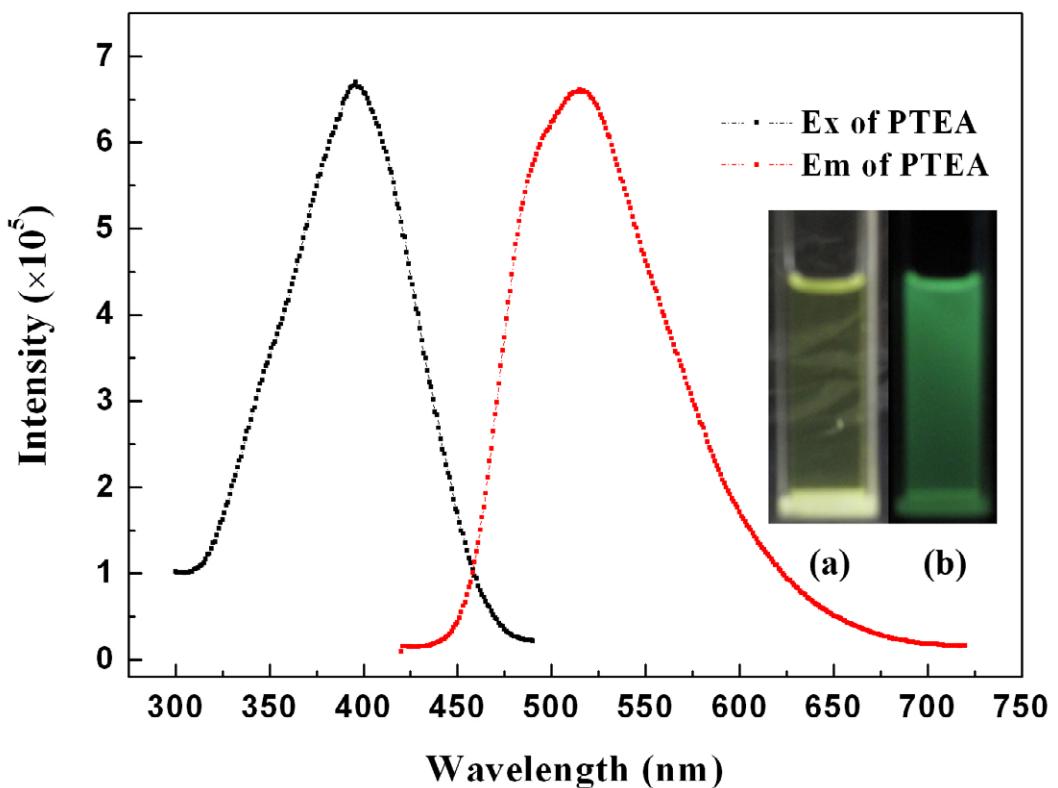
Details for the calculation of the detection limit of the fluorescent sensing film to picric acid in aqueous solution.

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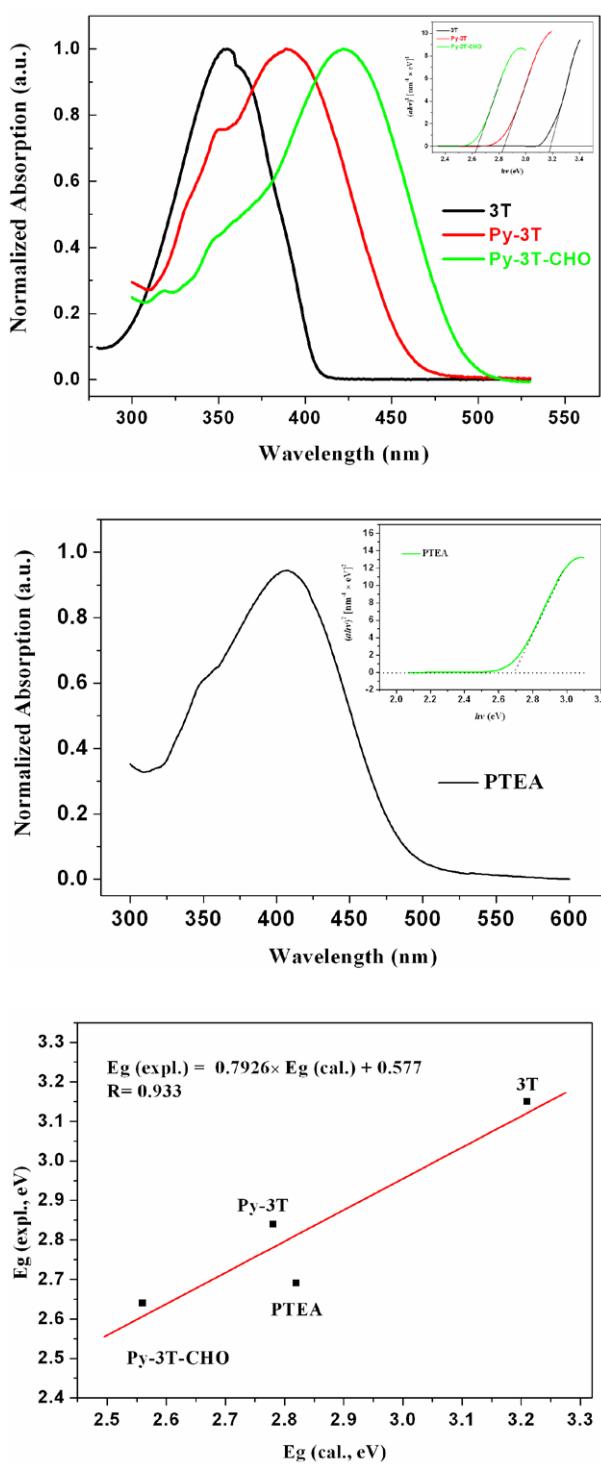
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Details for the calculation of the detection limit of the fluorescent sensing film to picric acid in aqueous solution.

Detection limit of the present film was determined and calculated according to the following functions:

$$s_b = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-1}} \quad (1)$$

$$S = \frac{\Delta I}{\Delta c} \quad (2)$$

$$DL = \frac{3s_b}{S} \quad (3)$$

Firstly, the standard deviation ( $s_b$ ) was calculated by measuring the intensity of the sensing film in blank solution for more than 10 times and then got the average intensity ( $\bar{x}$ ). By fitting the data into Function 1, the value of standard deviation ( $s_b$ ) was obtained. Secondly, a certain amount of picric acid (shown in Fig. 7) was added into the blank solution and the resulting variation of the intensity ( $\Delta I$ ) was recorded. By fitting the data into Function 2, where  $\Delta I$  is the variation of intensity, and  $\Delta c$  is the variation of quencher concentration, the value of precision  $S$  was calculated. Finally the detection limit,  $DL$ , was calculated according to Function 3.