Supporing Information for

Emission enhanced two-component gels for detection of organic amine vapors

Sisi Wang,[a,b] Pengchong Xue, [a] Panpan Wang, [a] Boqi Yao[a]

[a] Dr. P. Xue, P. Wang, B. Yao
College of Chemistry, Jilin University
No. 2519 Jiefang Road, Changchun (China)
E-mail: xuepengchong@jlu.edu.cn
[b] Dr. S. Wang
Institute of Translational Medicine
the First Hospital, Jilin University
Changchun (China)
Fig. S1 FT-IR spectra of C12Ph and the mixtures of C12Ph and SP at different ratios.
Fig. S2 TEM image of C12PhSP gel from cyclohexane.
Fig. S3 Normalized absorption spectra of C12PhSP gel in cyclohexane at different concentrations (cyclohexane of certain mL percent 1 mg C12PhSP).
Fig. S4 Absorption spectra of C12PhSP (C= 1.67 mg/mL) in wet gel and supernatant after centrifugation.
Fig. S5 Excitation spectra of C12PhSP during gelation and absorption spectrum of gel at room temperature. $\lambda_{em} = 450$ nm.
Fig. S6 Absorption spectral change of the mixture of C12Ph and SP with different molar ratios (a, 10:6; b, 10:3; c, 10:1) in cyclohexane (C = 1 mg/mL) from 80 to 20 °C.
Fig. S7 Absorption spectral change of the mixture of C12Ph and SP with different molar ratios (a, 10:6; b, 10:3, c, 10:1) in cyclohexane (C = 1 mg/mL) from 80 to 20 °C. λ_{em} = 340 nm.
Fig. S8 The time-course of fluorescence quenching of the xerogel film after being added into a cell filled with the vapors of aniline and n-butylamine; the intensity was monitored at 450 nm.
Fig. S9 Fluorescence spectra of the xerogel film before and after exposing to the saturated vapors of (a) N-methylaniline and (b) N,N-dimethylaniline for 30 s, and corresponding fluorescence after quenched film was exposed to air for 10 min. $\lambda_{ex} = 340$ nm.
Fig. S10 cycles of the PL quenching and recovery by exposing the nanofibril film to the saturated vapor of aniline (3s) and the air (5min), respectively.
Fig. S11 Fluorescence spectra of the xerogel film before and after exposing to the saturated vapors of (a) dibutylamine, (b) tributylamine, (c) diethylamine and (d) triethylamine for 30 s, and corresponding fluorescence after quenched film was exposed to air for 10 min. $\lambda_{ex} = 340$ nm.
Fig. S12 Absorption spectra of xerogel films upon exposure to aniline (a) and n-butylamine (b) vapors
Fig. S13 FT-IR spectra of C12PhSP xerogel film upon exposure to aniline and n-butylamine.
Table S1. The pKₐ and HOMO energy levels of amines and pyridine.

<table>
<thead>
<tr>
<th>amine</th>
<th>pKₐ</th>
<th>HOMO (ev)</th>
<th>amine</th>
<th>pKₐ</th>
<th>HOMO (ev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>aniline</td>
<td>9.37</td>
<td>-5.63</td>
<td>n-butylamine</td>
<td>3.41</td>
<td>-6.13</td>
</tr>
<tr>
<td>N-methylamine</td>
<td>9.15</td>
<td>-5.44</td>
<td>dibutylamine</td>
<td>3.35</td>
<td>-5.94</td>
</tr>
<tr>
<td>N,N-dimethylamine</td>
<td>8.93</td>
<td>-5.36</td>
<td>tributylamine</td>
<td>3.11</td>
<td>-5.60</td>
</tr>
</tbody>
</table>
### Table 1. The HOMO and LUMO energy levels of C12PhSP and SP.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>HOMO (eV)</th>
<th>LUMO (eV)</th>
<th>LUMO (eV)</th>
<th>HOMO (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SP</td>
<td>-5.59</td>
<td>-1.87</td>
<td>-1.80</td>
<td>-5.98</td>
</tr>
<tr>
<td>C12PhSP</td>
<td>-5.67</td>
<td>-1.95</td>
<td>-0.079</td>
<td>-6.26</td>
</tr>
</tbody>
</table>

*a* Electrochemical method was used to obtain the HOMO energy levels by comparing with an external reference, the ferrocene/ferrocenium (Fc/Fc⁺, 4.8 eV relative to vacuum).

*b* The LUMO energy level was estimated by subtracting $E_{\text{gap}}$ (3.72 eV) to $E_{\text{HOMO}}$.

*c* Energy levels of HOMO and LUMO versus vacuum were given after geometrical optimization at the B3LYP/6-31G level of theory.
Fig. S14 Fluorescence spectra of xerogel film upon exposure to common solvents.