Supporting Information

Luminescent Metal-Organic Frameworks Integrated Hydrogel Optical Fiber as a Photoluminescence Sensing Platform for Fluorescence Detection

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Fig. S1 (a) PXRD patterns of stimulated EuNDC, as-synthesized EuNDC, and EuNDC after immersing in deionized water and solutions of nitroaromatic compounds for 2 days. (b) TGA curve of EuNDC under the nitrogen atmosphere.

Fig. S2 (a) Injection of PEGDA precursor into the handmade mold with a syringe. (b) Polymerization of the PEGDA precursor under 365 nm irradiation. (c) Extraction out of the mold.

Fig. S3 Stimulated scattering loss versus particle sizes according to Mie scattering theory.
In the experiment, the particle sizes of EuNDC are in the range of 1-10 microns, and most of the particles concentrated at around 3 microns. So we assume the equivalent sphere diameter is about 3 microns. When the concentration of EuNDC is 0.25% w/v, the volume density (particle numbers per unit volume) of the particles is about 0.000004/μm³. The
wavelength in vacuum is 0.532 µm. The scattering angle is set to be 0°. The refractive index of the medium (PEGDA hydrogel) is 1.405, the refractive index of EuNDC is set to be 1.50.

Fig. S4 Photoluminescence spectrum of EuNDC incorporated hydrogel optical fiber under 365 nm LED irradiation.

Fig. S5 (a) Fluorescence image of the core of the hydrogel fiber immersed in 30 µM rhodamine B for 5 min. (b) Fluorescence image of the core of the hydrogel fiber immersed in 30 µM rhodamine B for 10 min. (c) Concentration distribution of rhodamine B along the diameter of the core after immersing in 30 µM rhodamine B for 5 min. (d) Concentration distribution of rhodamine B along the diameter of the core after immersing in 30 µM rhodamine B for 10 min.
The PEGDA cores of the hydrogel optical fiber are immersed in the 30 µM rhodamine B solution for 5 minutes and 10 minutes respectively, then the cores are dried under air (24°C, RH=70%) and cut across the transverse plane. The fluorescences of the labeled cores are observed by the fluorescence microscope.

Furthermore, the diffusion of rhodamine can be fitted by Fick’s law 1:

\[ C = C_0 (1 - \text{erf} \left( \frac{x}{2\sqrt{Dt}} \right)) \]

where \( \text{erf} (x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt \), and \( C_0 = 30 \, \text{µM} \), \( D = 0.0255 \, \text{mm}^2/\text{min} \).

Table S1 Energy levels of the HOMO and LUMO of the 4-NT, 2-NT, NB, 2,6-DNT, PA.

<table>
<thead>
<tr>
<th>Analytes</th>
<th>HOMO energy level [eV]</th>
<th>LUMO energy level [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA</td>
<td>-8.2374</td>
<td>-3.8978</td>
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<tr>
<td>4-NT</td>
<td>-7.3626</td>
<td>-2.3171</td>
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<tr>
<td>2-NT</td>
<td>-7.36454</td>
<td>-2.31722</td>
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<tr>
<td>NB</td>
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<td>-2.4283</td>
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<tr>
<td>2,6-DNT</td>
<td>-7.6448</td>
<td>-3.2877</td>
</tr>
</tbody>
</table>

Fig. S6 Fluorescence spectra of EuNDC in the presence of different solvents including water, ethanol, dimethylacetamide (DMA) and dimethylformamide (DMF).
Fig. S7 Excitation spectrum of EuNDC in the solid state monitored at the wavelength of 615 nm and photoluminescence spectrum of EuNDC in the solid state excited at the wavelength of 350 nm.

Fig. S8 (a) Fluorescence responses of EuNDC incorporated hydrogel optical fiber to NB in the range of 0-140 μL. (b) Fluorescence responses of EuNDC incorporated hydrogel optical fiber to 2,6-DNT in the range of 0-140 μL. (c) Fluorescence responses of EuNDC incorporated hydrogel optical fiber to 4-NT in the range of 0-140 μL. (d) Fluorescence responses of EuNDC incorporated hydrogel optical fiber to 2-NT in the range of 0-140 μL.
References