Supporting Information

for

Nanoconfinement of Tetraphenylethylene in Zeolitic Metal-Organic Framework for Turn-on Mechano fluorochromic Stress Sensing

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Figure S1. DFT simulation results of TPE monomer and its vibrations at 1073.98 cm$^{-1}$, 1233.80 cm$^{-1}$, 1436.83 cm$^{-1}$, and 1485.72 cm$^{-1}$. The infrared vibrational frequencies are obtained at the B3LYP/6-311G* level of theory and implementing an empirical scaling factor of 0.97.
**Figure S2.** ATR-FTIR spectra of TPE, TPE@ZIF-71 and ZIF-71. The predicted TPE spectrum was obtained from DFT calculations at the B3LYP/6-311G* level of theory and implementing an empirical scaling factor of 0.97.
Figure S3. TGA results of TPE, TPE@ZIF-71 and ZIF-71. The wt.% of TPE : ZIF-71 = (97.181 – 96.944) : 96.944 = 0.237 : 96.944
Figure S4. Solution $^1$H NMR of TPE@ZIF-71 where the guest/host peaks used for integration are indicated as TPE and dcIm, respectively. The guest loading calculated is 1 TPE for every 146 cages of ZIF-71.
Figure S5. The configuration of the TPE dimer calculated from DFT simulation and its maximum molecular size. The structure is obtained at the B3LYP-D3/6-311G* level of theory.
**Figure S6.** TPE/ZIF-71 pellet prepared using a physically-mixed powder of TPE and ZIF-71, and TPE@ZIF-71 pellet prepared under a nominal pressure of 346.6 MPa, their colors viewed in ambient light, and their fluorescence observed under a 365-nm UV lamp. The wt.% of TPE and ZIF-71 used to prepare the physically-mixed samples was based on the TGA results in Figure S3. Blue dots in the physically-mixed powders indicate the TPE molecules are not distributed uniformly, resulting in closer intermolecular interactions and a feeble caging effect, which allows for additional nonradiative decay channels and gives weak emission after pressure.
Figure S7. Peak positions of TPE@ZIF-71 and its pellets in the region of 490 – 590 cm⁻¹, as determined from Gauss fittings (in OriginPro).
Figure S8. Upper row: XRD patterns of TPE@MIL-68(In) and TPE@UiO-67; Lower row: TPE@MIL-68(In), TPE@UiO-67, and TPE@ZIF-71 pellets prepared under a nominal pressure of 346.6 MPa, their colors viewed in visible light (left), and their fluorescence under a 365 nm UV lamp (right).
Figure S9. Turn-on type mechanofluorochromic behavior of TPE@ZIF-71/PU fibers and TPE@ZIF-71/PVDF membranes. Note: the samples here are to demonstrate its sensing properties and engineering application potential. More rigorous research will be conducted as follow-on studies.
Table S1. Values of time constants ($\tau_i$), normalized pre-exponential factors ($a_i$), and fractional contributions ($c_i = \tau_i \cdot a_i$) of the emission decay of TPE suspension, ZIF-71 and TPE@ZIF71 powders upon excitation at 362.5 nm ($R_t = \sum a_i e^{-t/\tau_i}$, $R_t$ is the quantity/counts at time $t$).

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<th>Sample</th>
<th>$\lambda_{\text{obs}}$ [nm]</th>
<th>$\tau_1$ [ns]</th>
<th>$a_1$</th>
<th>$c_1$ [%]</th>
<th>$\tau_2$ [ns]</th>
<th>$a_2$</th>
<th>$c_2$ [%]</th>
<th>$\tau_3$ [ns]</th>
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<th>$c_3$ [%]</th>
<th>$\chi^2$</th>
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**Table S2.** Quantum yield (QY) of TPE suspension in a solution of water: THF = 99:1, ZIF-71 powder, TPE@ZIF-71 powder, and pellets.

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<tr>
<td>Pellet (86.65 MPa)</td>
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<td>Pellet (173.30 MPa)</td>
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<td>Pellet (346.60 MPa)</td>
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Table S3. Values of time constants ($\tau_i$), normalized pre-exponential factors ($a_i$), and fractional contributions ($c_i = \tau_i \cdot a_i$) of the emission decay of TPE@ZIF-71 pellets upon excitation at 362.5 nm.

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<th>Pelleting pressure [MPa]</th>
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<th>$a_1$</th>
<th>$c_1$ [%]</th>
<th>$\tau_2$ [ns]</th>
<th>$a_2$</th>
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Table S4. A comparison of the sensitivity of pure TPE versus TPE@ZIF-71. Note: when observed at the same peak wavelength, TPE@ZIF-71 only requires a nominal pressure of ~347 MPa, which is one-tenth of the pressure required for TPE at matching wavelength.

<table>
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