Solvatochromic fluorescent carbon dots as optic noses for sensing

volatile organic compounds

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EXPERIMENTAL SECTION

Materials. All the chemicals and solvents were purchased from commercial sources and used without further treatment, unless indicated otherwise.

General measurements.

Transmission electron microscopy (TEM) measurements were performed on a JEOL JEM-1011 transmission electron microscope. Size distributions and zeta potential measurement were performed using a Zetasizer Nano-ZS (Malvern Instruments Ltd.). UV-Vis absorption spectra were conducted on Shimadzu UV-2450 spectrophotometer. Photoluminescence spectra were conducted on PerkinElmer LS55. Proton nuclear magnetic resonance (¹H NMR) spectra were recorded on a Bruker AV 600 NMR spectrometer in deuterated chloroform (CDCl₃).

Synthesis of CDs.

The mixture of pCN-TPA (1.5 mg) and mPEG2k (200 mg) was dissolved in 10 mL of ethanol, and then the solution was transferred into a Teflon lined stainless autoclave. The sealed autoclave was heated to 100 °C and kept for 2 h. After cooling down, the crude product was purified by dialysis against deionized water and the final product was freeze-dried to yellow solid (150 mg).

Loading content of pCN-TPA in CDs.

The powder of CDs was dissolved in ethanol and analyzed with a UV–vis spectrophotometer at 394 nm by using a standard curve method. The loading content (LC) was calculated to be 0.57% by the following equation:

LC(wt%) = the weight of pCN-TPA in CDs/the weight CDs

Paper Sensor for Visual Detection of VOCs. The filter paper was cut into strips of 1 cm x 2.5 cm. The solution of CDs was casted on the strips, and then air dried naturally. The strip emitted strong orange fluorescence under the irradiation of 365 nm. Thereafter, the strips were exposed to the corresponding vaporized solvents for 30 s at room temperature and imaged under the illumination of 365 nm and the luminescent photos were taken by a digital camera.



Figure S1. The linear relationship between the concentration of pCN-TPA and absorption intensity at 394 nm in ethanol, the linear range is $0.5 - 50 \ \mu\text{g/mL}$ (R² = 0.9995) and the regression equation is y=0.00421x+0.00134.



Figure S2. The solubility of CDs in water (a) and organic solvent with concentration of 5 mg/mL (b).



Figure S3. The stability of CDs under irradiation and in different pH of solutions.



Figure S4. The PL spectra of CDs in the solvents of DCM (A), EA (B), THF (C), DMK (D), EtOH (E), MeOH (F), ACN (G), DMF (H) and water (I) under the excitation of different wavelengths.

CDs	H ₂ O	DMF	ACN	МеОН	EtOH	DMK	THF	EA	DCM
λ_{abs} (nm)	428	392	384	384	395	387	394	385	395
$\lambda_{ex,max}$ (nm)	320	340	340	340	340	340	340	340	340
$\lambda_{em,max} (nm)$	606	461	476	469	467	461	443	436	453
$\Phi_{\rm f}$ (%)	19.4	18.7	20.0	10.1	14.8	18.2	22.7	36.5	30.7
pCN-TPA	*H ₂ O	DMF	ACN	МеОН	EtOH	DMK	THF	EA	DCM
$\lambda_{abs} (nm)$		387	378	383	394	383	387	378	395
$\lambda_{ex,max} (nm)$		340	340	340	340	340	380	380	340
$\lambda_{em,max} (nm)$		457	504	445	445	459	630	624	639
$\Phi_{\rm f}$ (%)		2.5	2.6	2.0	2.7	2.7	7.6	22.0	10.1

 Table S1. Detailed absorption and emission peak positions of pCN-TPA in the different solvents.

*pCN-TPA is not soluble in water.