Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary data

Characterization of colorimetric sensor array by multi-spectral technique

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1. Colorimetric sensor array preparation

TiO_2 porous film was prepared by blending 3 g TiO_2 powder (P-25), 0.1 ml acetylacetone and 5 ml distilled water in a 35 ml agate mortar, and the mixture was stirred for 30 min. Then the mixture of 1.0 ml alcohol and 0.1 ml emulsification agents (octylphenylether polyethylene) was slowly added into the mortar with stirring continuously for 30 min. The TiO2 paste was spread onto the glass using a doctor blade scraping technique. Finally, the TiO2 nanoporous film was dried and sintered by firing the glass sheet at 450˚C in air for 4 h.

Certain amount of the selected dyes (0.1 M) were dissolved in chloroform or alcohol and printed on prepared TiO_2 porous film plate using microcapillary pipettes. Then these plates were dried in oven at 40˚C and maintained in dark and sealed condition.

2. Standard NH_3 generation

The NH3 permeation tube with NH3 liquor inside was the gas generation source. When fixed to the constant temperature bath, the volume of NH3 permeated through the tube wall for unit time become constant. At this time, additional supply of nitrogen (N2) as the dilution gas in a certain quantity generates standard gas with arbitrary micro-concentration which will be stabilized for a long time. The concentration of the NH3 vapor in the stream of N2 can be obtained by the following formula:

$$C = \frac{K \times \mathrm{Pr} \times L}{F} \qquad (1)$$

where C is the concentration of NH3 (ppm). Pr is the permeation rate (134 ng/min/cm). L is the effective length of tube (10 cm). F is the flow rate of nitrogen (ml/min). K is the factor to convert the weight to volume of the gas (1.44 L/g). Furthermore, the different humidity levels (%RH) were created by controlling the feeding of mixing nitrogen/water vapors at different ratio.

Phenolphthalein	Methyl orange	Bromocresol green	Bromocresol purple
Screened methyl orange (first transition)	Malachite green (second transition)	Bromothymol blue	Naphtholphthalein
5,10,15,20-Tetraphenyl-21H,23H-porphine cobalt(II)	5,10,15,20-Tetraphenyl-21H,23H-porphine	5,10,15,20-Tetrakis(4-methoxyphenyl)-21H,23H-porphine	Screened methyl orange (second transition)
Zinc 2,3,9,10,16,17,23,24-octakis(octyloxy)-29H,31H-phthalocyanine	Zinc 5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine	Zinc 29H,31H-tetrabenzo[b,g,l,q] porphine	5,10,15,20-Tetraphenyl-21H,23H-porphine manganese(III) chloride

Fig.S1 Dyes used for colorimetric sensor array

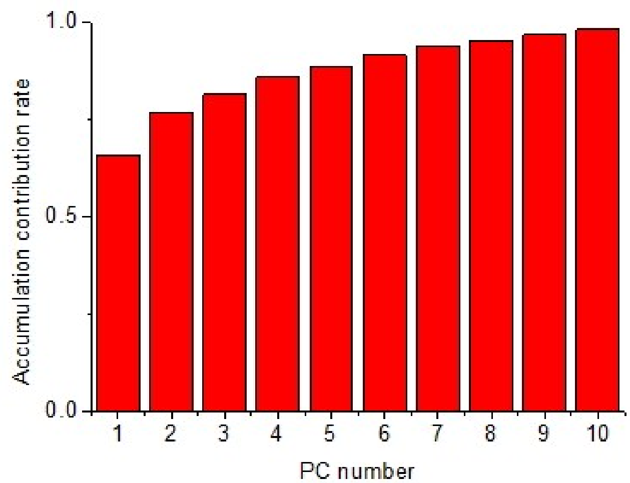

Fig.S2 Cumulative contributions of the top 10 PCs.

Table S1. The optimum characteristic wavelengths for all 16 dyes and the transmission wavelengths of the filters used for each dye.

Name	Optimum characteristic wavelengths(nm)	Used filters
Bromocresol purple	794, 828, 530	BP540/10K, BP808/10K, BP935/30K
Naphtholphthalein	791, 830, 939	BP619/10K, BP808/10K, BP935/30K
Methyl orange	619, 809, 931	BP619/10K, BP808/10K, BP935/30K
Phenolphthalein	620, 799, 933	BP619/10K, BP808/10K, BP935/30K
Naphtholphthalein	689, 789, 941	BP619/10K, BP808/10K, BP935/30K
Bromothymol blue	663, 838, 933	BP619/10K, BP808/10K, BP935/30K

Malachite green (second transition)	550, 626, 934	BP540/10K, BP619/10K, BP935/30K
Screened methyl orange (first transition)	797, 840, 938	BP619/10K, BP808/10K, BP935/30K
Screened methyl orange (second transition)	613, 828, 936	BP619/10K, BP808/10K, BP935/30K
5,10,15,20-Tetrakis(4-methoxyphenyl)-21H,23H-porphine	603, 788, 935	BP619/10K, BP808/10K, BP935/30K
5,10,15,20-Tetraphenyl-21H,23H-porphine	605, 792, 932	BP619/10K, BP808/10K, BP935/30K
5,10,15,20-Tetraphenyl-21H,23H-porphine cobalt(II)	611, 799, 921	BP619/10K, BP808/10K, BP935/30K
5,10,15,20-Tetraphenyl-21H,23H-porphine manganese(III) chloride	589, 789, 938	BP619/10K, BP808/10K, BP935/30K
Zinc 29H,31H-tetrabenzo[b,g,l,q] porphine	797, 885, 934	BP619/10K, BP808/10K, BP935/30K
Zinc 5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine	534, 826, 909	BP540/10K, BP808/10K, BP935/30K
Zinc 2,3,9,10,16,17,23,24-octakis(octyloxy)-29H,31H-phthalocyanine	786, 540, 941	BP540/10K, BP808/10K, BP935/30K