Supplementary Information for

Photochromic Spiropyran-Embedded PDMS for Highly Sensitive and Tunable Optochemical Gas Sensing

Yoon-Seung Nam[a], Imsung Yoo[b], Oktay Yarimaga[a], In Sung Park[a], Dong-Hoon Park[a], Simon Song*[b,c], Jong-Man Kim*[a,c] and Chan Woo Lee*[c]

[a] Department of Chemical Engineering, Hanyang University, Seoul 133-791, Korea. E-mail: jmk@hanyang.ac.kr.

[b] Department of Mechanical Engineering, Hanyang University, Seoul 133-791, Korea. E-mail: simonsong@hanyang.ac.kr

[c] Institute of Nano Science and Technology, Hanyang University, Seoul 133-791, Korea. E-mail: lcw@hanyang.ac.kr

Experimental

A typical procedure for a spiropyran-embedded PDMS film preparation is as follows. A methylene chloride (0.1 mL) solution containing 10 mg of 1,3,3-trimethylindolino-6'-nitrobenzopyrylospiran (SP) (Sigma-Aldrich) was injected into a mixture (22 g) of PDMS elastomer base (Sylgard 184) and PDMS curing agent (DC184A, weight ratio = 10:1). After gentle shaking for 30 min, the mixture was poured into a petridish (diameter: 3.5 cm) and cured at 70 ^{o}C for 2 h to give a colorless film (thickness: 2.2 mm). The thickness of the film can be controlled by choosing a proper size of the dish.

The spiropyran containing PDMS microfluidic chip was fabricated using the following procedure. A PDMS prepolymer mixture was obtained by injecting methylene chloride solution (0.1 mL) of spiropyran (5 mg) into a mixture (11 g) of dimethylsiloxane and initiator (weight ratio = 10:1). After degassing in a vacuum chamber for 30 min, the mixture was poured onto the mold and cured in an oven at 70 ^{o}C for 2 h. The patterned PDMS substrate

was peeled from the mold, washed with isopropyl alcohol, and bonded to a glass slide. The chip was irradiated with 365 nm UV light for 3 min before use.

Fluorescent images were obtained using a fluorescence microscope (IX71, Olympus) with a 4x objective and a color charge-coupled device (CCD) camera (DP71, Manufacturer). The flow rates of the HCl gas were controlled by using a syringe pump (KDS120, KD Scientific).

Pressure Calculation

Because Reynolds number for the HCl gas flow with a maximum flow rate of 5 mL/h is 2.1, all HCl flows are laminar and pressures at measurement points in the microchannel can be estimated by using the Poiseuille flow relationship,

$$\frac{\Delta p}{\Delta x} = \frac{8\mu}{\pi R^4} Q$$

where Q is the flow rate and Δx is the length (0.8 cm) between the measurement point to the outlet subject to atmospheric pressure. Also, R is the hydraulic radius (33.33 μm) and μ is the viscosity of HCl gas (0.00014 g/cms). Table S1 shows pressures and effective diffusivities of HCl for six flow rates.

Table S1

Flow rate (mL/h)	0	1	2	3	4	5
Effective diffusivity ($\mu m^2/s$)	22.80	237.02	521.90	702.26	829.62	943.18
Pressure (Pa)	0	64.2	128.4	192.6	256.8	321

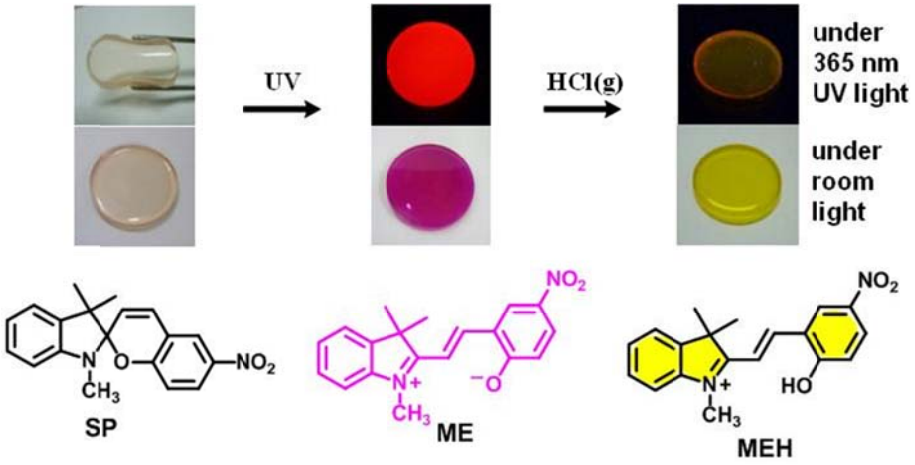

Figure S1. Color and fluorescence changes of a spiropyran-embedded PDMS film in response to UV and HCl(g).

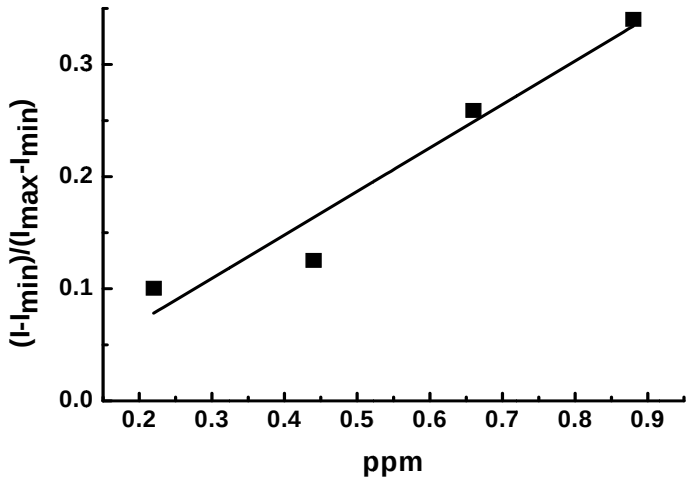

Figure S2. Plots yellow intensity of as a function of HCl concentration.

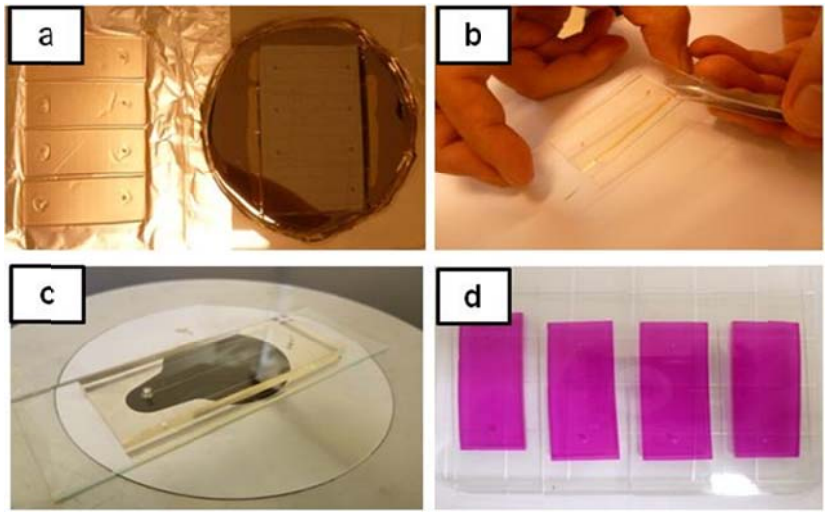

Figure S3. Preparation of a microfluidic chip with spiropyran-embedded PDMS substrates (a: spiropyran-containing PDMS molding, b: PDMS bonding to a glass substrate, c: a microfluidic chip before UV irradiation, d: microfluidic chips after 365 nm UV irradiation for 3 min (1 mW/cm^2)).

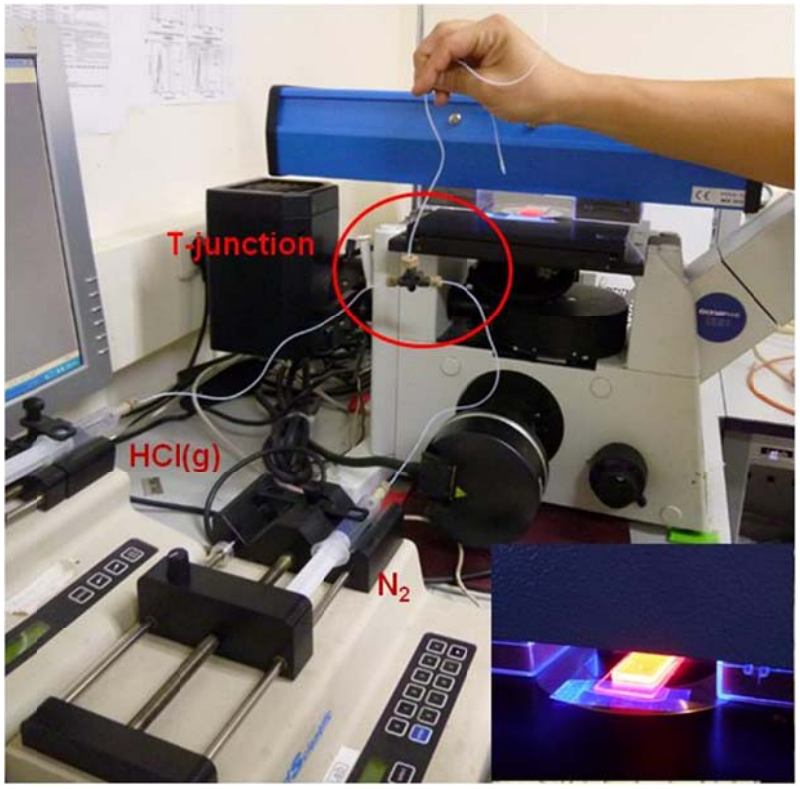

Figure S4. Experimental set-up.

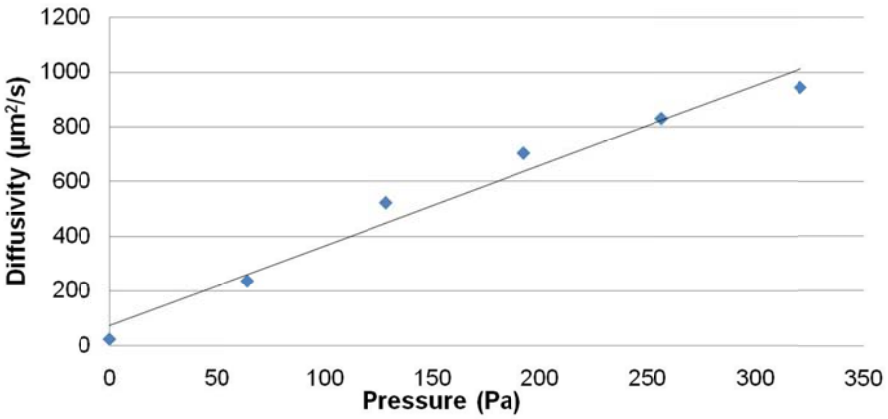

Figure S5. Plots of effective HCl diffusivity in spiropyran-embedded PDMS as a function of pressure. The line is a linear fit of the data.

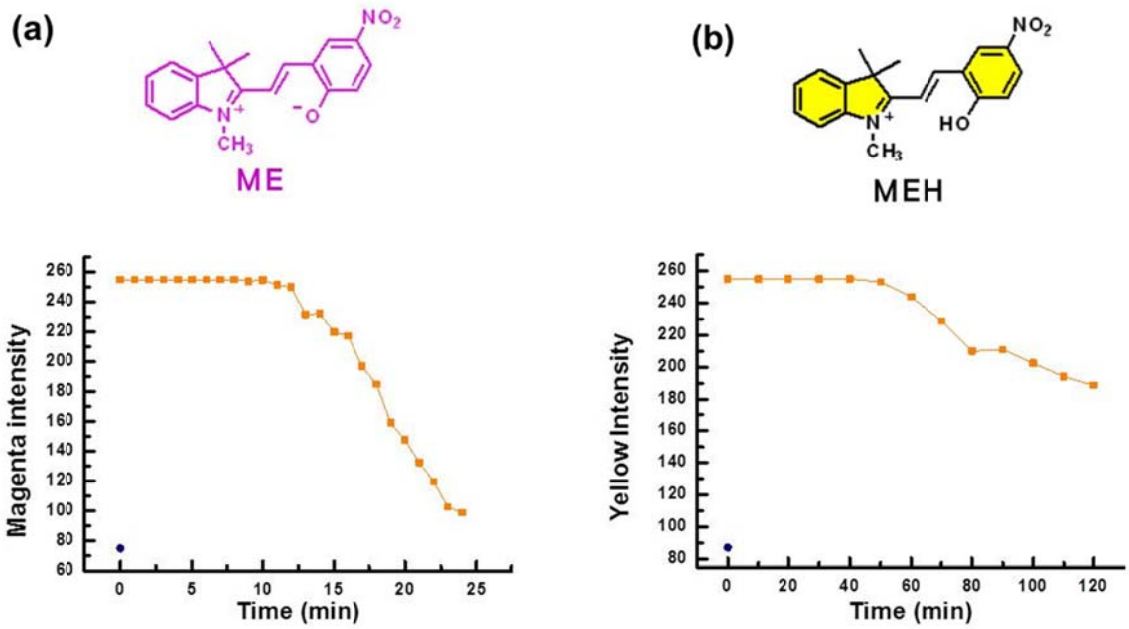

Figure S6. Plots of magenta (a) and yellow (b) intensity as a function of time for ME (a) and MEH (b) forms of the photochromic compound.

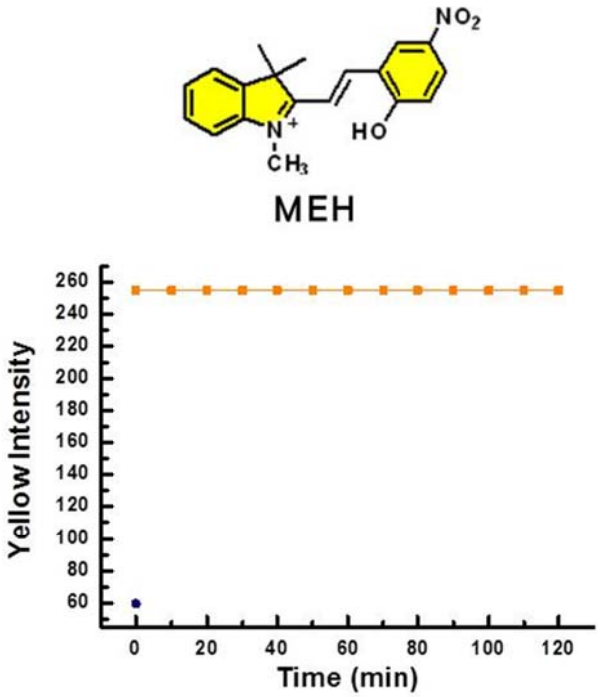

Figure S7. Plots of yellow intensity as a function of time for MEH form during 365 nm UV irradiation.

References

S1. J. M. Kim, E. K. Ji, S. M. Woo, H. Lee and D. J. Ahn, *Adv. Mater.*, 2003, **15**, 1118-1121.