

Surface-Enhanced Infrared Absorption: Pushing the Frontier for On-Chip Gas Sensing

Xinyuan Chong,¹ Yujing Zhang,² Erwen Li,¹ Ki-Joong Kim,^{3,5} Paul R. Ohodnicki,^{3,4} Chih-Hung (Alex) Chang² and Alan X. Wang^{1,*}

¹ School of Electrical Engineering and Computer Science, Oregon State University, Corvallis, OR 97331, USA

² School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR 97331, USA

³ National Energy Technology Lab, United States Department of Energy, Pittsburgh, PA 15236, USA

⁴ Materials Science and Engineering Department, Carnegie Mellon University, Pittsburgh, PA 15213, USA

⁵ AECOM, P.O. Box 618, South Park, PA 15216, USA

*Corresponding author: wang@eecs.oregonstate.edu

Numerical Simulation

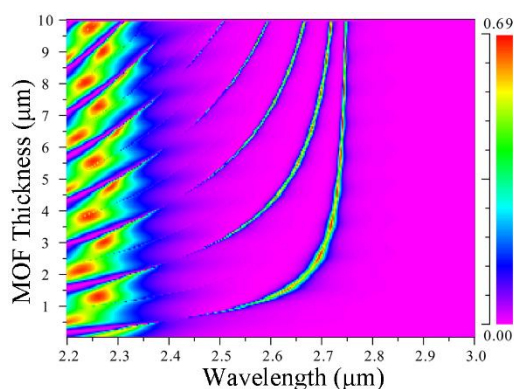


Figure S1. The scanning of MOF thickness.

The scanning of MOF thickness is shown in Figure S1, with all other parameters fixed. The color bar indicates the transmission intensity. The mode around 2.7 μm is the mode M_t at the top Au/MOF/Air interface, which will be cutoff when the MOF thickness is less than 500 nm. As the thickness increases, more high-order modes will appear.

Characterization

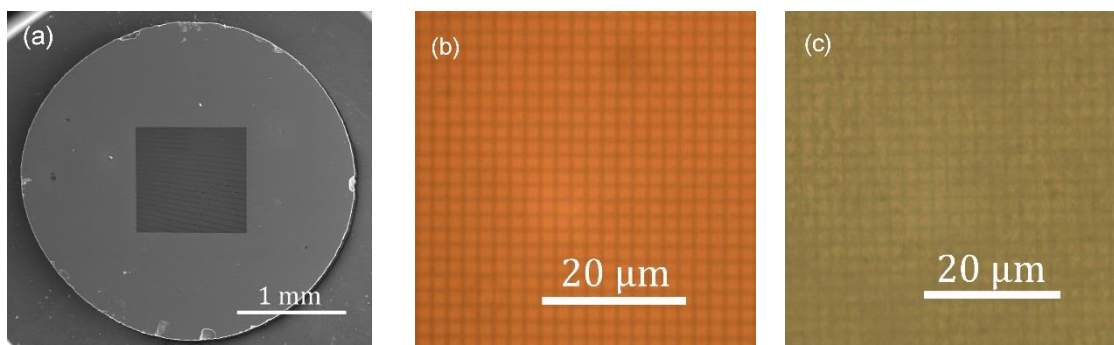


Figure S2. (a) The SEM image of the Si_3N_4 nano-membrane on Si wafer. The optical images of Au-NPA (b) before and (c) after coating MOF.

The SEM image of Si_3N_4 nano-membrane on Si wafer is shown in Figure S2 (a). The optical images of Au-NPA before and after coating MOF are shown in Figure S2 (b) and S2 (c).

Experiment

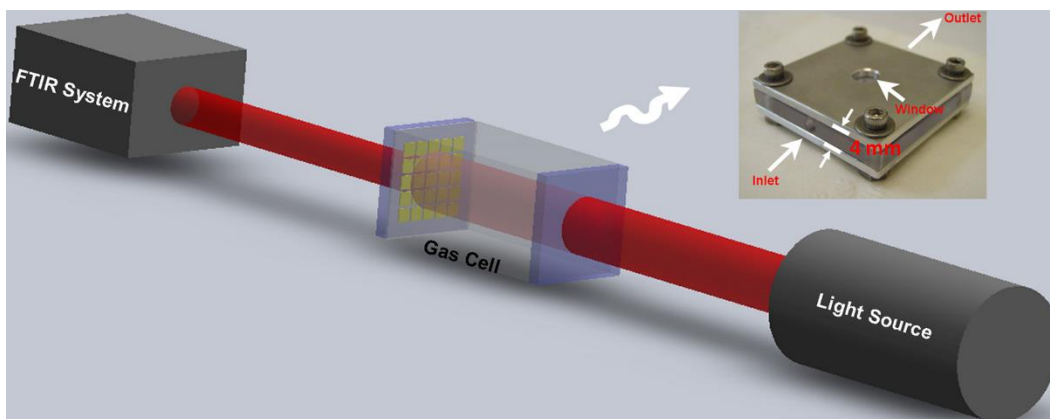


Figure S3. The schematic of the testing system with a home-made gas cell

The quantitative CO_2 absorption measurement was performed by a commercial Fourier transform infrared (FTIR) spectrometer. A home-made gas cell was used in the test, which has 4 mm path length as shown in Figure S3. One side of the gas cell is sealed by a sapphire window and the other side is sealed by the device.

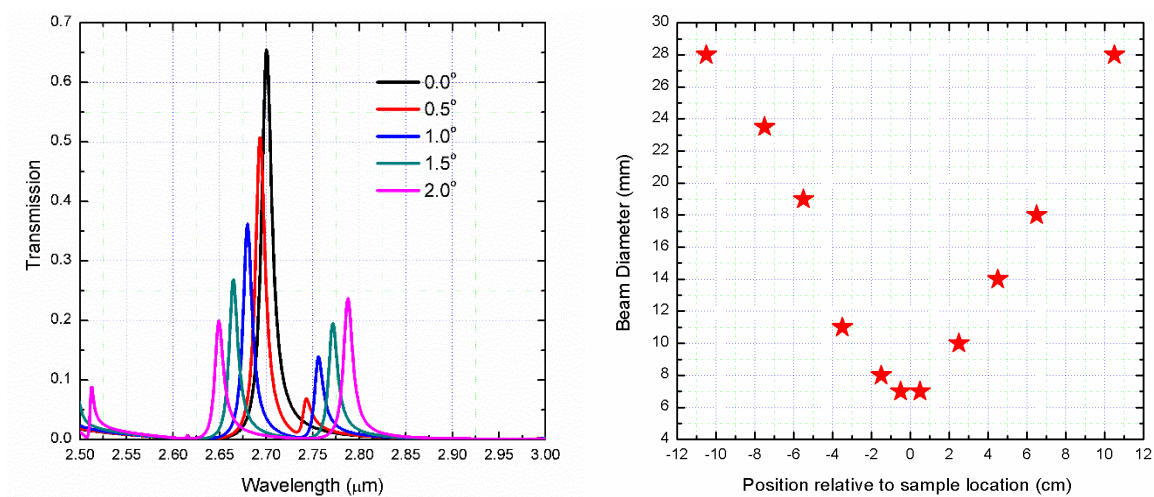


Figure S4. (a) The effect of incident angle deviation. (b) Beam diameter of FTIR.

The simulated transmission spectra of the device with different incident angles are shown in Figure S4 (a). We also measured the beam diameter of our commercial FTIR spectrometer. A tunable aperture was placed at different positions along the beam path. As shown in Figure S4 (b),

the beam diameter varies rapidly along the optical path, indicating a low quality of beam collimation. The non-collimated beam contains light with a broad range of spatial angles and will cause broadening of the transmission spectrum and lower the transmission efficiency.

Data Analysis

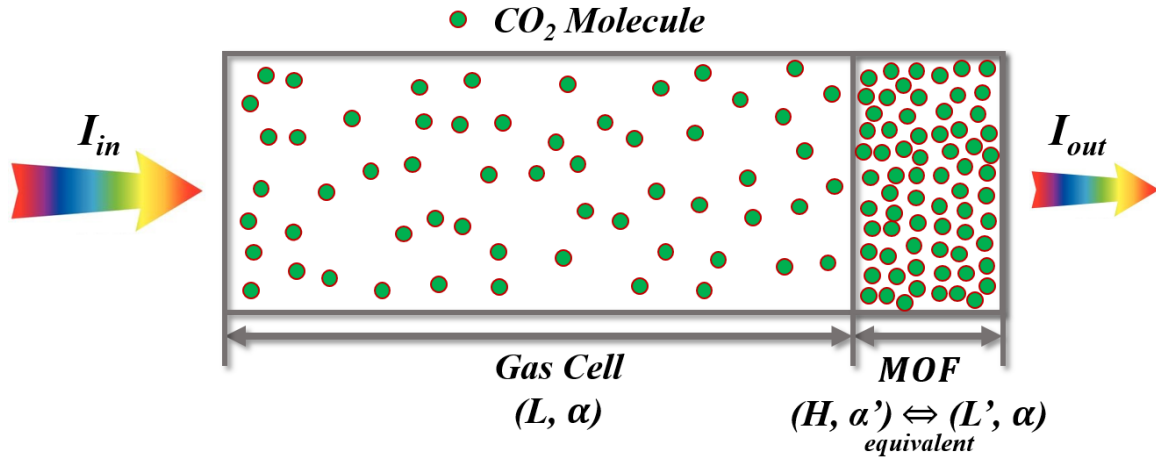


Figure S5. Illustration of data analysis.

In order to determine the enhancement caused by MOF and plasmonics, an analysis was performed as illustrated in Figure S5. For the bare sapphire window sample, since there is no enhancement, the absorption is purely from CO₂ in the gas cell. Therefore, the actual absorption coefficient α of CO₂ can be calculated from this sample based on Beer-Lambert law:

$$I_{out} / I_{in} = \exp(-\alpha \cdot L) \quad (1)$$

where L is the path length of the gas cell. For the other two sample, besides the CO₂ in the gas cell, there are extra CO₂ molecules adsorbed inside the MOF. The absorption can be expressed as:

$$I_{out} / I_{in} = \exp(-\alpha \cdot L - \alpha' \cdot L') \quad (2)$$

where α' is the absorption coefficient of the CO₂ adsorbed inside MOF layer, which is larger than α .

Equation (2) can be rewritten as:

$$I_{out} / I_{in} = \exp[-\alpha \cdot (L + L'')] \quad (3)$$

where L'' is effective enhanced absorption length, induced by MOF layer. The actual thickness of MOF layer is H . Therefore, the enhancement factor is defined as $EF = L'' / H$.