Supplementary Information: Standoff mechanical resonance spectroscopy based on infrared sensitive hydrogel microcantilevers

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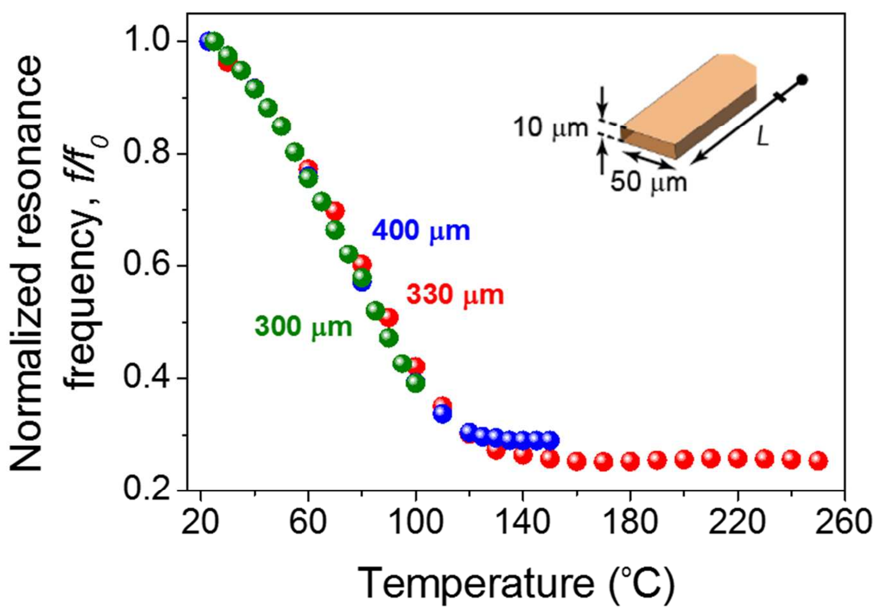
A. Thermal response of PEG-DA microcantilevers

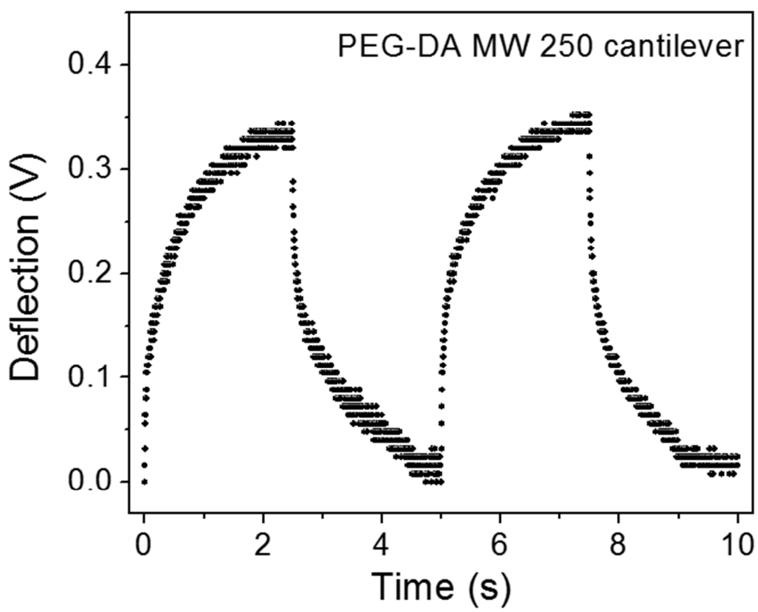
Fig. S1 shows the normalized resonance frequency shifts of 300, 330, and 400 μm long PEG-DA microcantilevers that are heated on the microceramic heater. The resonance frequency of PEG-DA microcantilever decreases until the temperature of ~120 °C, and it reaches a thermally insensitive phase. The three different microcantilevers were fabricated from the same material, PEG-DA MW 250 in one batch, and thus they show the same trend in normalized resonance frequency shift upon heating. The resonance frequency of each PEG-DA microcantilever restored back to the initial f_0 when the cantilever cooled down to room temperature.



Supplementary Figure S1. Normalized resonance frequencies of the PEG-DA microcantilevers with 3 different lengths (L) (green: 300 μm, red: 330 μm, blue: 400 μm) as a function of temperature. The width and thickness of the cantilevers are 50 μm and 10 μm as shown in the inset.

B. Deflection of the PEG-DA microcantilever in static mode

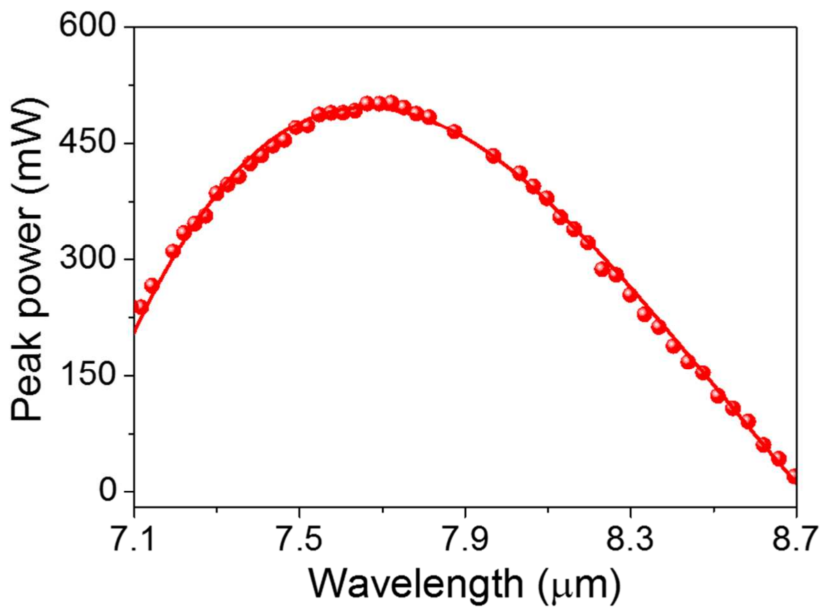
In order to measure the static response of PEG-DA microcantilever to IR, pulsed IR of 0.2 Hz at the wavelength of 7.76 μm is irradiated on one side of the microcantilever which has a 20/100-nm thick metal (Ti/Au) coating on the opposite side. As the PEG-DA microcantilever absorbs IR, molecular vibrations are excited and generate heat. This heat expands both the PEG-DA and metal layers. Due to the difference in thermal expansion coefficients of these layers, the PEG-DA microcantilever bends. A low pulsing frequency of 0.2 Hz helps the microcantilever in achieving the saturation state. From the measured data of static deflection, time constant is obtained, ~0.5 seconds.



Supplementary Figure S2. Deflection profile of a PEG-DA MW 250 microcantilever in static mode as a response to the pulsed IR of 0.2 Hz.

C. Peak power curve of UT-8 QCL

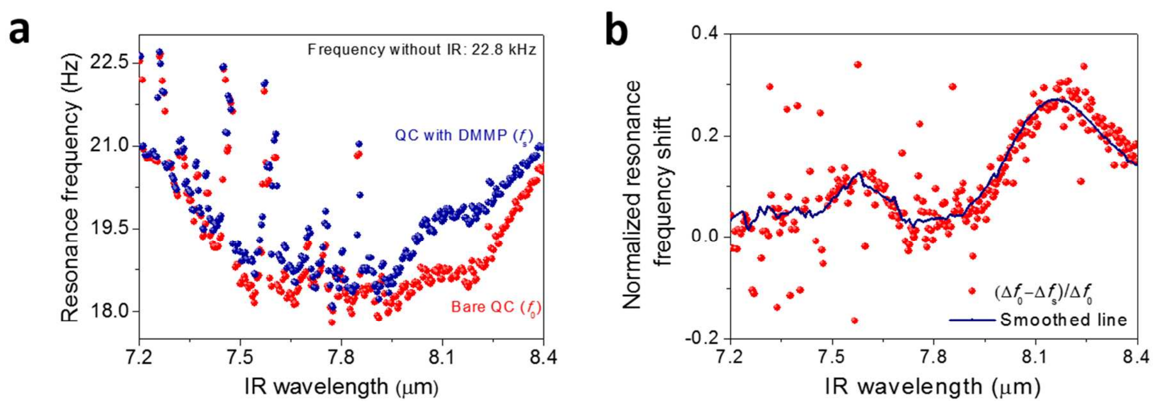
The peak power profile of the UT-8 QCL at 1100 mA current, provided by Daylight Solutions, Inc. (San Diego, CA) is shown in Fig. S3. It depends on the wavelength; it increases when the wavelength changes from 7.1 to 7.7 μm and then decreases when the wavelength further increases from 7.7 to 8.7 μm.



Supplementary Figure S3. Wavelength-dependent peak power profile of the UT-8 QCL at 1100 mA.

D. Data processing for the standoff spectrum (fractional method)

The fractional method is used to process the standoff spectra in the main manuscript as shown in Fig. S4. In this fractional method, the difference in the resonance frequency shift of the PEG-DA microcantilever with and without the sample (Δf_s–Δf_0) is divided by the resonance frequency shift without the sample (Δf_0). The result called the normalized frequency shift difference provides the normalized sensor responses[S1]. As an example, Fig. S4a and S4b show resonance frequency shifts of the PEG-DA with and without the DMMP (Δf_s and Δf_0) and the fractional frequency shift ((Δf_s–Δf_0)/Δf_0), respectively. Finally, the normalized frequency shift difference data is smoothed. The intensity ratios of two peaks located at 7.6 and 8.14 μm are 0.5 for the frequency shift difference (Δf_s–Δf_0) and 0.35 for the normalized frequency shift difference ((Δf_s–Δf_0)/Δf_0), respectively. The latter value shows better agreement with the intensity ratio from the reference FTIR measurement (0.37).



Supplementary Figure S4. (a) Resonance frequency changes of the PEG-DA MW 250 microcantilever (length, width, and thickness: 300, 50, and 10 μm) as a function of the wavelength of the pulsed IR illumination, which is reflected off the QC surface with (f_s)

and without (f_0) DMMP. (b) DMMP standoff spectrum processed using the fractional method and smoothing.

References

S1. Hines, E. L., Llobet, E. & Gardner, J. W. Electronic noses: a review of signal processing techniques. *IEE Proc. - Circuits, Devices Syst.* **146,** 297 (1999).