Identification and Quantitative Detection of Two Pathogenic Bacteria based on Terahertz Metasensor

Zhaofu Ma,^{†ab} Yanan Jiao,^{†ab} Chiben Zhang,^{†c} Jing Lou,^{bc} Pengyue Zhao,^a Bin Zhang,^a Yujia Wang,^a Ying Yu,^c Wen Sun,^d Yang Yan,^a Xingpeng Yang,^a Lang Sun,^b Ride Wang,^b Chao Chang,^{*b} Xiru Li,^{*a} and Xiaohui Du,^{*a}

*Corresponding Authors: Xiaohui Du, E-mail: duxiaohui301@sina.com; Xiru Li, E-mail: 2468li@sina.com; Chao Chang, E-Mail: gwyzlzssb@pku.edu.cn.

Supplementary Note 1

Simulated effect of 10-nm thick titanium on resonance

After adding the titanium layer, we find that the amplitude and frequency of the resonance merely change marginally, as shown in Fig S1(a). Quantitatively, the frequency-shift (Δf) and amplitude-modulation (Δa) are 4 GHz and 0.0017, respectively, as shown in Fig S1 (b). Thus, adding 10 nm-thick titanium has little effect on the resonance of the metasurface.



Fig S1. (a) Simulated transmission spectra of metasurface with/without titanium layer. (b) Enlarged view of the black wireframe.

Supplementary Note 2

Effect of other structural parameters on the resonance

The effect of distance (b) between SSRs and CW on the coupling of the two dipoles is simulated, as shown in Fig. S2(a). Fig. S2(b) and (c) show the variation of the Q factor and resonance intensity with different b for two modes, respectively. As the b increases, the frequency range of the resonance narrows and the Q factor increases for mode II, while the Q factor and resonance intensity both decrease for mode I.

As shown in Fig. S2(d), we simulated the constructive and destructive hybridizations of the two dipoles with different cut size (c) of SRRs. Fig. S2(e) and (f) show the variation of the Q factor and resonance intensity with different c for two modes, respectively. With the increase of the cut

size of SRRs, the Q factor decreases for mode I, and the Q factor increases for mode II, while the resonance undergoes blueshift.

Based on the above simulation results, the *b* was set as 2 μ m to ensure the high Q property of mode I and to compare the differences between the detection results of two modes in the frequency domain. The *c* mainly affects the *Q* factor of two modes, while it has trifling impact on resonance intensity. Thus, we set *c* as 2 μ m to enable the mode I with high *Q* property.



Fig. S2 The designed metasurface and resonant properties extracted from simulations. (a) Simulated transmission spectra with different distances between SSRs and CW. (b) Q factor and (c) resonance intensity variations of two modes with different distances between SSRs and CW, with the other parameters fixed. (d) Simulated transmission spectra with different cut sizes of SRRs. (e) Q factor and (f) resonance intensity variations of two modes with different cut size of SRRs, with the other parameters fixed.

Supplementary Note 3

Micrographs of samples with different concentrations on the metasensor

5×10^4 cfu/mL			$1 \times 10^5 cfu/mL$			$5 \times 10^5 cfu/mL$			$1 \times 10^6 cfu/mL$		
(a)00	00	00	GG(d)	00	00	(°) (°)	80	1930		6	8
00	000	00	69	8	<u>e</u>	<u></u>	8	8	8	00	8
00	00	00	90	8	00		<u>.</u> 201	8	8		00
(e) 00	00	00		0j0	GD	(8))	00	99	(h)	00	8
00	00	00	00	000	8	80	60	8		8	e,
00	60	00	60	00	8	00	80	60	ġ.	0	00

Fig. S3. Optical micrographs of (a-d) Escherichia coli, (e-f) Staphylococcus aureus deposited onto the THz metasensor, with four concentrations including 5×10^4 cfu/mL, 1×10^5 cfu/mL, 5×10^5 cfu/mL, and 1×10^6 cfu/mL, respectively.

Supplementary Note 4

Measured sensing performances of the mode II in application

Fig. S4(a) and (b) show the transmission spectra of two bacteria with different concentrations, and the insets reveal the enlarged views of blue wireframes. As the concentration of bacteria increases, the mode II shifts to low frequency, and its amplitude changes irregularly. Fig. S4(c) shows the extracted frequency-shift of two bacteria with different concentrations for mode II. The frequency-shift of mode II is slightly smaller than that of mode I. With the bacterial concentration increasing, the irregular amplitude changes occur in the mode II, especially for the detection of Escherichia coli, as shown in Fig. S4(d).

In the proposed metasurface, the mode I is generated by the constructive interference of the toroidal dipole on the electric dipole, as well as the mode II is formed by the cancellation of the two dipoles. Furthermore, the low Q factor (13.85) and weak resonance intensity of the mode II imply low accuracy for the detection and data processing. Thus, we choose the detection results of mode I for analysis to obtain accurate and minor biological information in practical application.



Fig. S4 Measured sensing performances of the mode II. Experimental transmission spectra of (a) Escherichia coli and (b) Staphylococcus aureus with different concentrations. Extracted (c) frequency-shift and (d) relative amplitude-modulation of two bacteria with different concentrations for two modes. The error bar represents standard deviations calculated from three measurements.