Electronic Supplementary Information

Ultrasensitive Trace-Analyte Detection Empowered by a Flexible Quasi-BIC Terahertz Metasensor

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1. Experimental setup

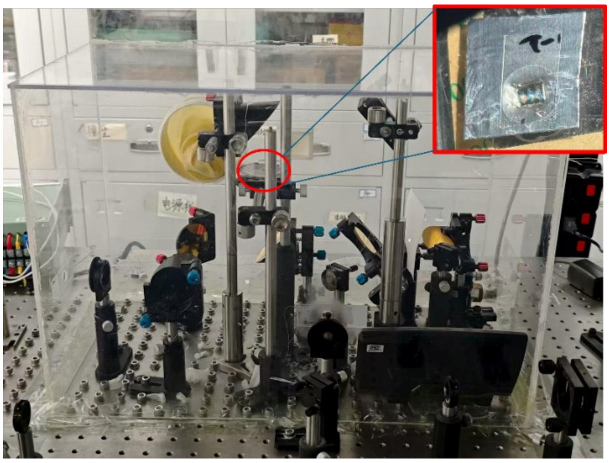

Fig. S1 Photograph of the customed terahertz time-domine spectroscopy. Insert: sample holder and the metamaterial sample covered by aluminum foil.

2. Relative permittivity of copolymers of cycloolefin (COC) dielectric materials

To acquire the complex permittivity of COC substrate, we perform a transmissive measurement using the terahertz time-domain spectroscopy (THz-TDS) system. By performing a Fourier transform on measured time-domain signals, the transmission spectra of the COC thin film with a thickness of 50μm and corresponding reference signal through the free-space are obtained in the frequency domain. The complex permittivity of the COC film can be extracted from the measured data based on following equations [1]

$$\begin{aligned} &\tilde{\varepsilon} = \varepsilon_r(1+\tan\delta) = \tilde{n}^2 = (n_r + ik)^2 \\ &T(\omega) = \frac{E_s(\omega)}{E_r(\omega)} = |T(\omega)| \cdot \exp[i\varphi(\omega)] \\ &n_r(\omega) = 1 - \frac{c}{\omega d} \cdot \varphi(\omega) \\ &k(\omega) = \frac{c}{\omega d} \cdot \ln\left[\frac{(n_r(\omega)+1)^2}{4n_r(\omega)} \cdot |T(\omega)|\right] \end{aligned} \qquad (S1)$$

where k and $\tan\delta$ are the extinction coefficient and loss tangent, respectively, d refers to the thickness of the COC film. $E_s(\omega)$ and $E_r(\omega)$ are complex transmission spectra measured with and without the COC film. In Fig. S2, we present the frequency-dependent permittivity and loss tangent in the frequency range of 0.4 – 1.0 THz.

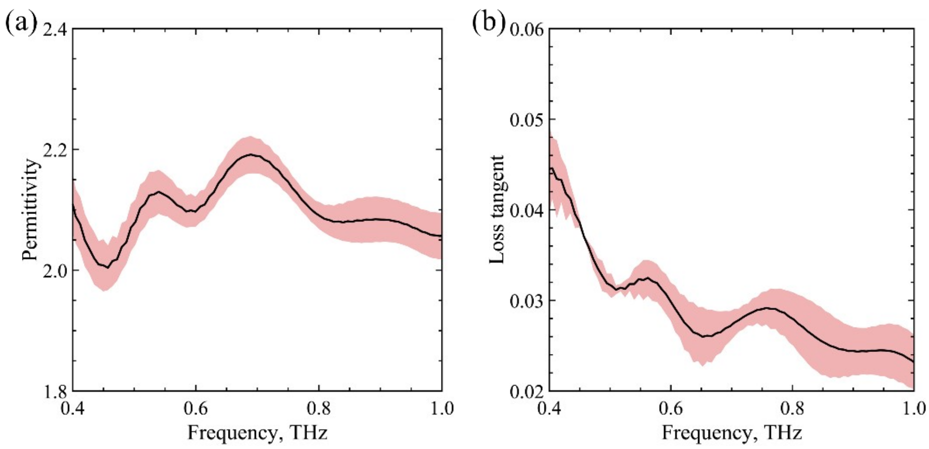

Fig. S2 (a) Permittivity and (b) loss tangent of COC film. The shaded band denotes the standard deviation obtained from multipole experimental trials.

3. Fano modelling of the simulated transmission curves

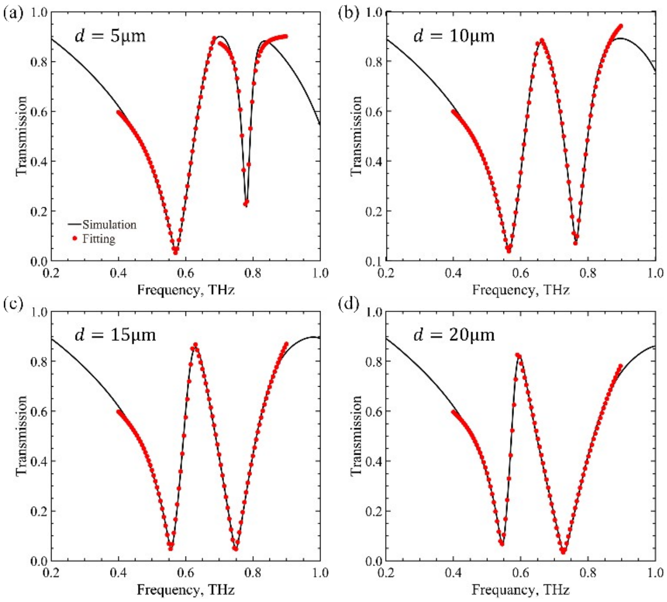

Fig. S3 Simulated and Fano-fitting curves of metamaterials with different asymmetric parameters.

4. Temporal coupled mode theory analysis

The dynamic tuning of the quasi-BIC resonance in our metamaterial can be captured with a framework of the temporal coupled mode theory, which are governed by [2]

$$\frac{d}{dt}\begin{bmatrix}a_1\\a_2\end{bmatrix} = (j\Omega-\Gamma)\begin{bmatrix}a_1\\a_2\end{bmatrix}+K\begin{bmatrix}s_{1+}\\s_{2+}\end{bmatrix} = j\begin{bmatrix}\omega_{01}+j\gamma_1 & k+j\gamma_{12}\\ k+j\gamma_{21} & \omega_{02}+j\gamma_2\end{bmatrix}\begin{bmatrix}a_1\\a_2\end{bmatrix}+\begin{bmatrix}k_{11}&k_{12}\\k_{21}&k_{22}\end{bmatrix}\begin{bmatrix}s_{1+}\\s_{2+}\end{bmatrix} \quad (S2)$$

where a_1 and a_2 are the resonant amplitudes of resonant modes, ω_{01} and ω_{02} are their resonant frequencies, γ_1 and γ_2 are their decay rates, k represents the coupling rate between two modes, $\gamma_{12}=\gamma_{21}$ is the coupling coefficient generated by the damping. k_{ij} $(i,j=1,2)$ is the coupling coefficient between tow modes, s_{1+} and s_{2+} are the input wave amplitudes from two input ports. The output waves are given by

$$\begin{bmatrix}s_{1-}\\s_{2-}\end{bmatrix} = \begin{bmatrix}r_d & t_d\\ t_d & r_d\end{bmatrix}\begin{bmatrix}s_{1+}\\s_{2+}\end{bmatrix}+\begin{bmatrix}d_{11}&d_{12}\\d_{21}&d_{22}\end{bmatrix}\begin{bmatrix}a_1\\a_2\end{bmatrix} \quad (S3)$$

where s_{1-} and s_{2-} are outgoing waves amplitudes, r_d and t_d are the direct reflection and transmission coefficient between two ports without resonant modes. d_{ij} $(i,j=1,2)$ is the coupling coefficient between two ports. Based on the energy conservation, these coefficients can be simplified as $k_{11}=k_{12}=|d_{11}|=|d_{12}|=\sqrt{\gamma_1}$ and $k_{21}=k_{22}=|d_{21}|=|d_{22}|=\sqrt{\gamma_2}$. Solving these equations, we can obtain the amplitude of these two modes as

$$\begin{aligned} a_1(\omega) &= \frac{jk-\gamma_{12}}{j(\omega-\omega_{01})+\gamma_1}a_2(\omega)+\frac{\gamma_1}{j(\omega-\omega_{01})+\gamma_1}s_{1+}(\omega) \\ a_2(\omega) &= \frac{(jk-\gamma_{12})\sqrt{\gamma_1}+[j(\omega-\omega_{01})+\gamma_1]\sqrt{\gamma_2}}{[j(\omega-\omega_{01})+\gamma_1][j(\omega-\omega_{02})+\gamma_2]-(jk-\gamma_{12})^2}s_{1+}(\omega) \end{aligned} \quad (S4)$$

The outgoing amplitude at Port 2 is

$$s_{2-}(\omega) = t_d s_{1+}(\omega) - \left[\sqrt{\gamma_1}a_1(\omega)+\sqrt{\gamma_2}a_2(\omega)\right] \quad (S5)$$

Thus, the complex transmission coefficient can be calculated by

$t_{21}(\omega) = s_{2-}(\omega)/s_{1+}(\omega) \qquad (S6)$

Quality factors of these two modes can be expressed in terms of the decay rates as $Q_m = \omega_{0m}/2\gamma_m$ with $m = 1, 2$.

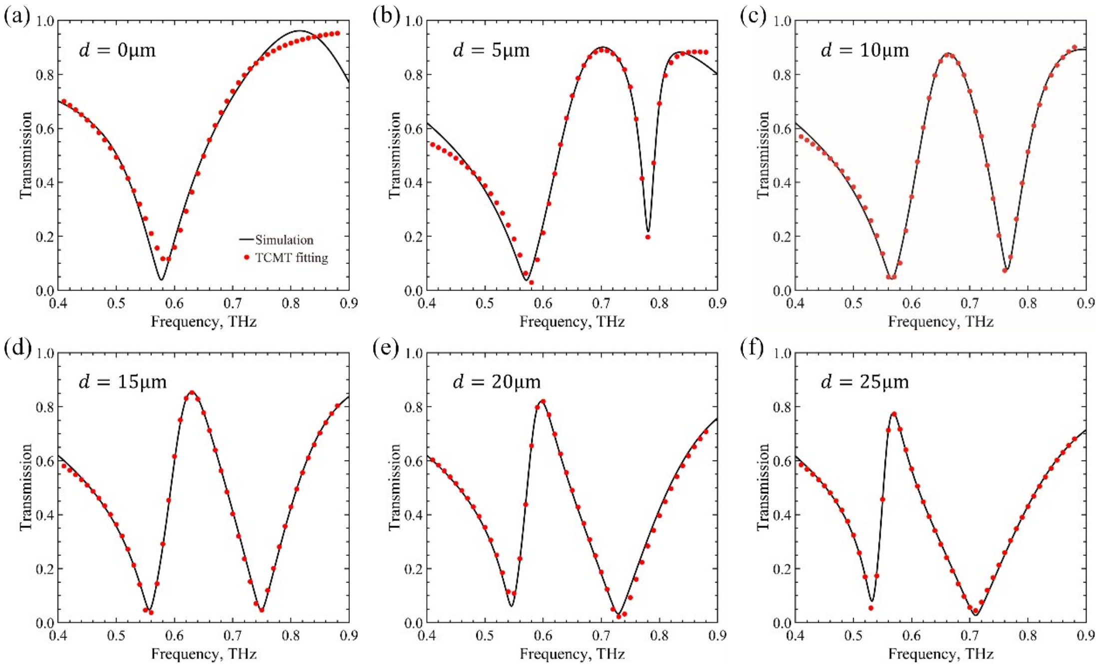

Fig. S4 Comparison of transmission spectra for the proposed metamaterial between simulations (black solid lines) and TCMT calculations (red dotted lines) with (a) $d = 0\mu m$, (b) $d = 5\mu m$, (c) $d = 10\mu m$, (d) $d = 15\mu m$, (e) $d = 20\mu m$ and $d = 25\mu m$.

Table S1 Fitting parameters for the proposed metamaterial based on TCMT modeling.

d (μm)	ω_{01} ($\times 2\pi\, THz$)	γ_1 ($\times 2\pi\, THz$)	ω_{02} ($\times 2\pi\, THz$)	γ_2 ($\times 2\pi\, THz$)	k ($\times 2\pi\, THz$)
0	0.578	0.120	-	-	-
5	0.571	0.099	0.781	0.020	0.182
10	0.566	0.084	0.764	0.067	0.170
15	0.557	0.065	0.749	0.140	0.168
20	0.545	0.053	0.729	0.210	0.159
25	0.532	0.038	0.710	0.340	0.154

[1] K. Im, S. Kim, Y. Cho, Y. Woo, C. Chiou, THz-TDS Techniques of Thickness Measurements in Thin Shim Stock Films and Composite Materials, Applied Sciences 11(19), (2021), 8889.

[2] X. Zhao, C. Chen, K. Kaj, I. Hammock, Y. Huang, R.D. Averitt, X. Zhang, Terahertz investigation of bound states in the continuum of metallic metasurfaces, Optica 7 (11) (2020) 1548–1554.