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Spectral and temporal evidence of robust photonic bound states in the continuum on terahertz metasurfaces: supplementary material

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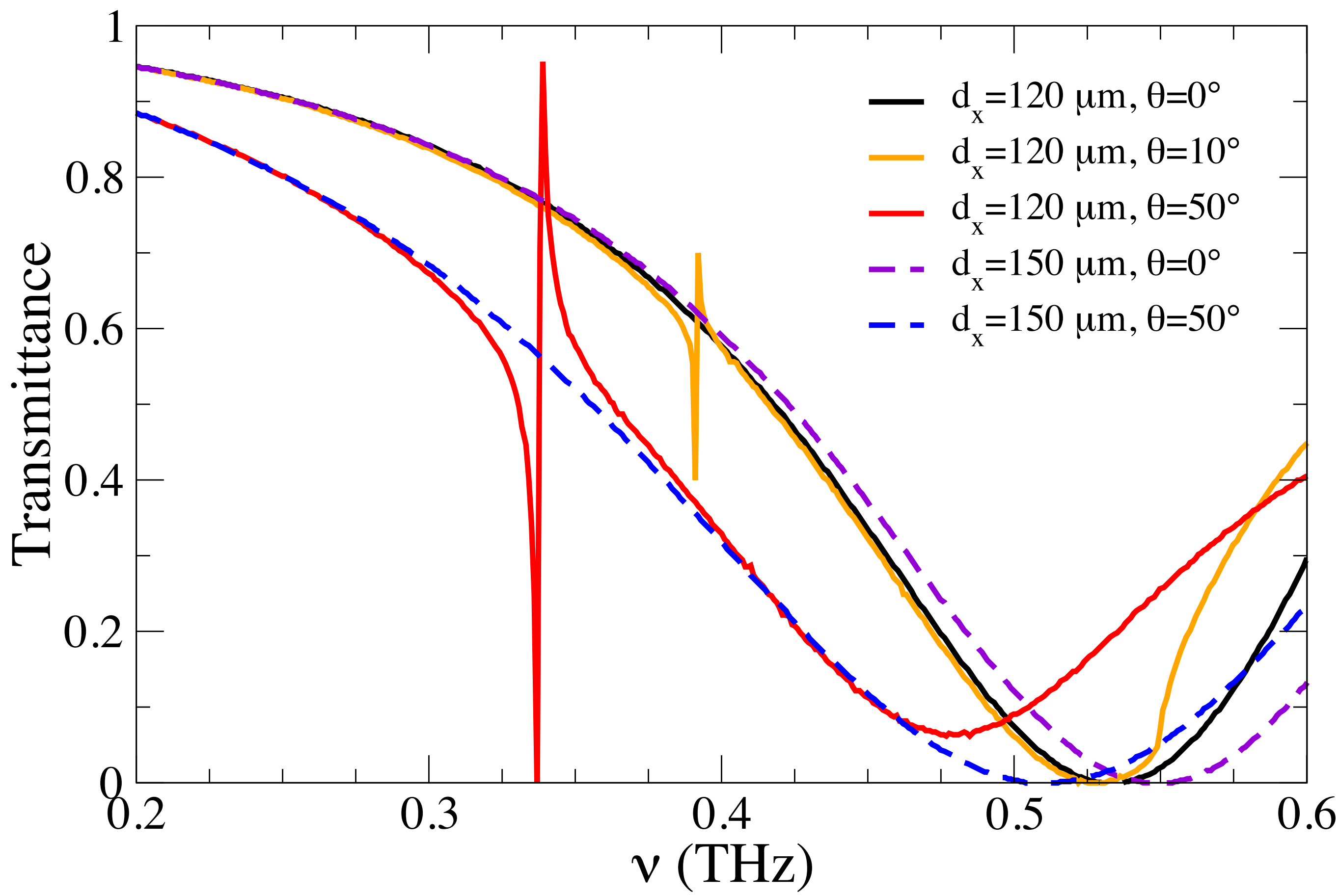

Fig. S1. Transmittance spectra numerically calculated through SCUFF for a plane wave incident at $\theta = 0°, 50°$ on a square lattice ($a = 300\ \mu$m) of two planar gold rods per unit cell embedded in a uniform medium with $n = 1.55$, with two different rod separations: $d_x = a/2$ (dashed curves) and $d_x = 2a/5$ (solid curves), in the latter case, $\theta = 10°$ is also considered to further illustrate the emergence of a Fano resonance. Gold rods are identical and have dimensions $L_1 = L_2 = 200\,\mu$m and $w_1 = w_2 = 40\,\mu$m.

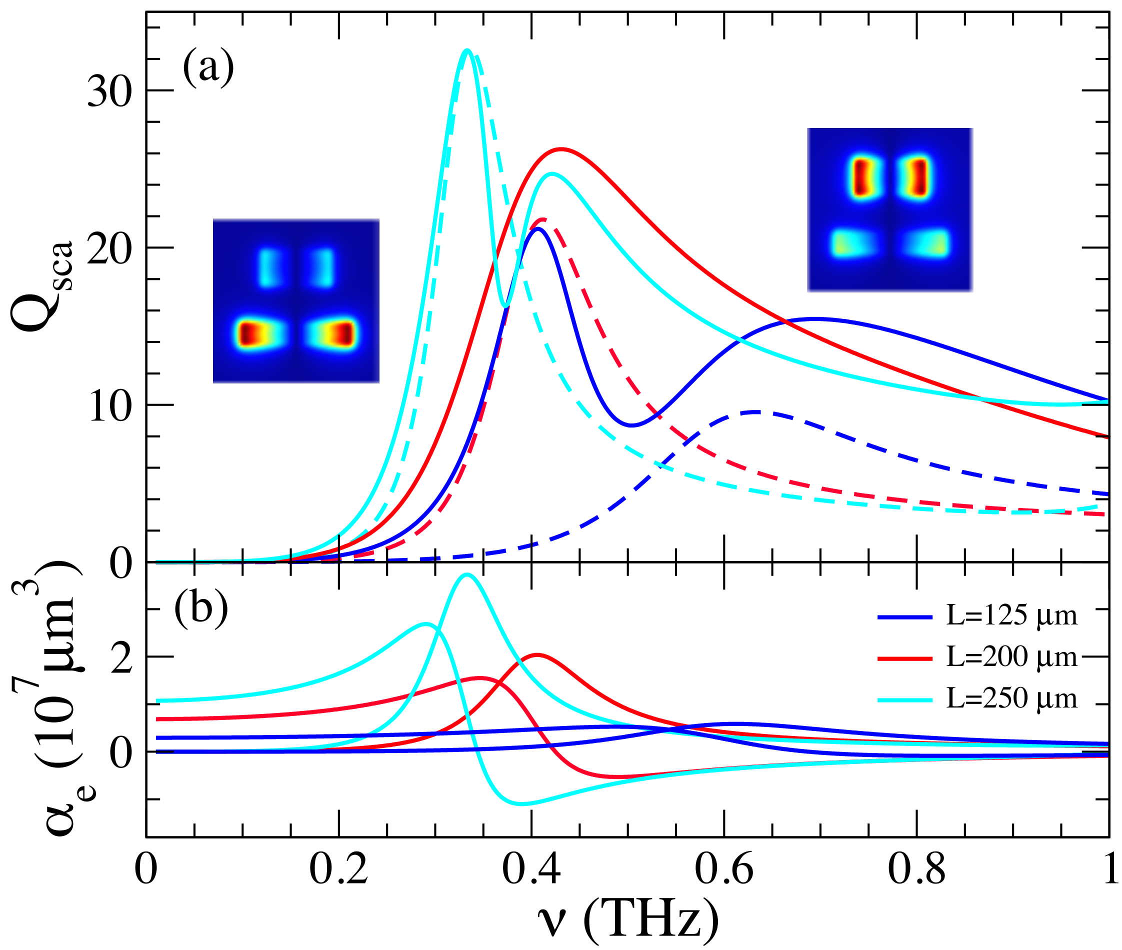

Fig. S2. (a) Scattering efficiencies (solid curves) numerically calculated through SCUFF for perfectly conducting planar dimer rods (separated by $d = 120\ \mu$m) with lengths $L_1 = 200\ \mu$m and: $L_2 = 125, 200$ and 250 μm (widths satisfy $w(\mu\mathrm{m}) = 8000/L$). Corresponding efficiencies for single isolated rods with $L = L_2$ are also included (dashed curves). Insets show the near-field maps (magnetic field perpendicular to the dimer plane) for the dimer with $L_2 = 125\mu$m at the two resonances. Significant interference between rods is observed in the dimer spectra, which do not correspond to simply a linear combination of the isolated spectra of each rod. Rather, rod interference leads to a stronger/weaker impact of the higher/lower frequency rod resonance (apart from their opposite phases, not shown), as expected. (b) Real and imaginary parts of the polarizibilities of the single rods extracted from (a). In order to avoid numerical problems related to unphysical absorption, we consider in our coupled dipole model that dipoles are lossless so that the imaginary parts of the polarizabilities are fixed to $\Im\left[1/\alpha_y^{(i)}\right] = -k^3/(6\pi)$ to fulfill the optical theorem, taking for the real parts the values calculated numerically.

1. COUPLED DETUNED-DIPOLE FORMULATION

First of all, let us define the scalar Green function, $g(\mathbf{r}-\mathbf{r_n})$, resulting from the Helmholtz equation with a point source located at $\mathbf{r}=\mathbf{r_n}$:

$$\nabla^2 g + k^2 g = -\delta(\mathbf{r}-\mathbf{r_n}), \tag{S1}$$

whose solution is

$$g(\mathbf{r}-\mathbf{r_n}) = \frac{e^{\imath k|\mathbf{r}-\mathbf{r_n}|}}{4\pi k|\mathbf{r}-\mathbf{r_n}|}k. \tag{S2}$$

The Weyl expansion of the scalar Green function is

$$g(\mathbf{r}-\mathbf{r_n}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dQ_x dQ_y}{4\pi^2} e^{\imath Q_x(x-x_n)} e^{\imath Q_y(y-y_n)} \frac{\imath}{2q} e^{\imath q|z-z_n|}, \qquad q=\sqrt{k^2-Q_x^2-Q_y^2}. \tag{S3}$$

The element yy of the (tensor) Green function, $G_{yy}(\mathbf{r}-\mathbf{r_n})$, is

$$\begin{aligned} G_{yy}(\mathbf{r}-\mathbf{r_n}) &= \left(1+\frac{1}{k^2}\frac{\partial^2}{\partial y^2}\right) g(\mathbf{r}-\mathbf{r_n}) \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dQ_x Q_y}{4\pi^2}\left(1-\frac{Q_y^2}{k^2}\right) e^{\imath Q_x(x-x_n)} e^{\imath Q_y(y-y_n)} \frac{\imath}{2q} e^{\imath q|z-z_n|}. \end{aligned} \tag{S4}$$

This element will be needed below.

Next, let us consider a 2D periodic lattice of two detuned dipoles per unit cell in the xy plane. The lattice has a rectangular symmetry with pitch a and b in the x and y-axis, respectively, while the separation between the dipoles in the unit cell is d_x and d_y along the x and y-axis, respectively. The (parallel) dipoles are characterized by their polarizabilities along the y-axis, $\alpha_y^{(1)}$ and $\alpha_y^{(2)}$, where (1) and (2) account for each dipole in the unit cell. The array is excited by an external plane wave, ψ_0, polarized along the y-axis and with wavevector $\mathbf{k}=k_z\hat{\mathbf{z}}+k_x\hat{\mathbf{x}}$. The dipole positions (1) and (2) are

$$\mathbf{r_{nm}^{(1)}} = (-d_x/2+na)\hat{\mathbf{x}} + (-d_y/2+mb)\hat{\mathbf{y}}, \tag{S5}$$

$$\mathbf{r_{nm}^{(2)}} = (d_x/2+na)\hat{\mathbf{x}} + (d_y/2+mb)\hat{\mathbf{y}}. \tag{S6}$$

From now on, we refer to the set of dipoles defined by $(n,m)=(0,0)$ as the central dipoles, placed at $\mathbf{r_{00}^{(i)}}\equiv\mathbf{r^{(i)}}$, with $i=1,2$. The y component of the field at the position of the central dipoles, $\psi_{loc}^{(i)}$, is the sum of the waves scattered from the rest of particles plus the external plane wave:

$$\begin{aligned} \psi_{loc}^{(1)}(\mathbf{r^{(1)}}) &= \psi_0^{(1)}(\mathbf{r^{(1)}}) + k^2\alpha_y^{(1)}\sum_{nm}{}'\left[G_{yy}\left(\mathbf{r^{(1)}}-\mathbf{r_{nm}^{(1)}}\right)\psi_{loc}^{(1)}(\mathbf{r_{nm}^{(1)}})\right] + k^2\alpha_y^{(2)}\sum_{nm}\left[G_{yy}\left(\mathbf{r^{(1)}}-\mathbf{r_{nm}^{(2)}}\right)\psi_{loc}^{(2)}(\mathbf{r_{nm}^{(2)}})\right], \\ \psi_{loc}^{(2)}(\mathbf{r^{(2)}}) &= \psi_0^{(2)}(\mathbf{r^{(2)}}) + k^2\alpha_y^{(1)}\sum_{nm}\left[G_{yy}\left(\mathbf{r^{(2)}}-\mathbf{r_{nm}^{(1)}}\right)\psi_{loc}^{(1)}(\mathbf{r_{nm}^{(1)}})\right] + k^2\alpha_y^{(2)}\sum_{nm}{}'\left[G_{yy}\left(\mathbf{r^{(2)}}-\mathbf{r_{nm}^{(2)}}\right)\psi_{loc}^{(2)}(\mathbf{r_{nm}^{(2)}})\right], \end{aligned} \tag{S7}$$

where $\sum_{nm}$ runs over n,m and $\sum_{nm}{}'$ means that the sum runs for all indices except for $(n,m)=(0,0)$.

From Bloch's theorem, the local fields are related to the field at the central dipoles as

$$\psi_{loc}^{(i)}(\mathbf{r_{nm}^{(i)}}) = \psi_{loc}^{(i)}(\mathbf{r^{(i)}})e^{\imath k_x na}. \tag{S8}$$

Thus, Eq. (S7) in matricial form reads

$$\begin{bmatrix}\psi_{loc}^{(1)}\\ \psi_{loc}^{(2)}\end{bmatrix} = \begin{bmatrix}\psi_0^{(1)}\\ \psi_0^{(2)}\end{bmatrix} + k^2\begin{bmatrix}G_{byy} & G_{yy}^{(1-2)}\\ G_{yy}^{(2-1)} & G_{byy}\end{bmatrix}\begin{bmatrix}\alpha_y^{(1)} & 0\\ 0 & \alpha_y^{(2)}\end{bmatrix}\begin{bmatrix}\psi_{loc}^{(1)}\\ \psi_{loc}^{(2)}\end{bmatrix}, \tag{S9}$$

where the position dependence $(\mathbf{r^{(i)}})$ is assumed and suppressed, and

$$\begin{aligned} G_{byy} &= \sum_{nm}{}' G_{yy}\left(\mathbf{r^{(i)}}-\mathbf{r_{nm}^{(i)}}\right)e^{\imath k_x na}, \\ G_{yy}^{(1-2)} &= \sum_{nm} G_{yy}\left(\mathbf{r^{(1)}}-\mathbf{r_{nm}^{(2)}}\right)e^{\imath k_x na}, \\ G_{yy}^{(2-1)} &= \sum_{nm} G_{yy}\left(\mathbf{r^{(2)}}-\mathbf{r_{nm}^{(1)}}\right)e^{\imath k_x na}. \end{aligned} \tag{S10}$$

From Eq. (S9) it is easy to solve for the local fields (Eq. (1)) once we determine the lattice green dyadic, as follows.

Combining the Poisson summation formula:

$$\frac{2\pi}{a}\sum_l \delta\left(K-\frac{2\pi l}{a}\right) = \sum_n e^{\imath Kan}, \tag{S11}$$

with the Weyl expansion of the Green function, Eq. (S4), the term $G_{yy}^{(i-j)}$ can be rewritten as:

$$G_{yy}^{(1-2)} = \sum_{lp} \frac{\imath}{2k_{zlp}ab}\left(1-\frac{k_{yp}^2}{k^2}\right) e^{-\imath k_{xl} d_x} e^{-\imath k_{yp} d_y},$$
$$G_{yy}^{(2-1)} = \sum_{lp} \frac{\imath}{2k_{zlp}ab}\left(1-\frac{k_{yp}^2}{k^2}\right) e^{\imath k_{xl} d_x} e^{\imath k_{yp} d_y}, \tag{S12}$$

with

$$k_{xl} = k_x - \frac{2\pi l}{a}, \qquad k_{yp} = -\frac{2\pi p}{b}, \qquad k_{zlp} = \sqrt{k^2 - k_{xl}^2 - k_{yp}^2}. \tag{S13}$$

At normal incidence, $k_x = 0$ and $G_{yy}^{(1-2)} = G_{yy}^{(2-1)}$ reading as:

$$G_{yy}^{(1-2)} = \frac{\imath}{2k_z ab} + 4\sum_{l=1}^{\infty}\sum_{l=p}^{\infty} \frac{\imath}{2k_{zlp}ab}\left(1-\frac{k_{yp}^2}{k^2}\right)\cos\left(k_{xl}d_x\right)\cos\left(k_{yl}d_y\right) \tag{S14}$$

Thus, in the absence of diffraction its imaginary part is

$$\Im\left[G_{yy}^{(1-2)}\right] = \frac{1}{2k_z ab}. \tag{S15}$$

Similarly, using the Weyl expansion the term G_{byy} can be written as:

$$G_{byy} = \lim_{z\to 0}\left[\sum_{lp} \frac{\imath}{2k_{zlp}ab}\left(1-\frac{k_{yp}^2}{k^2}\right) e^{\imath k_{zlp}|z|} - G_{yy}(z\hat{\mathbf{z}})\right], \tag{S16}$$

where the term $(n,m) = (0,0)$ has been also included in the sum. Although the real part is intricate (the real parts of both terms in Eq. (S16) diverge), the imaginary part is well behaved

$$\Im\left[G_{byy}\right] = -\frac{k}{6\pi} + \sum_{lp}^{prop} \frac{1}{2k_{zlp}ab}\left(1-\frac{k_{yp}^2}{k^2}\right), \tag{S17}$$

where the sum runs for all propagating orders $\left(\Im\left[k_{zlp}\right] = 0\right)$.

Finally, for lossless particles the imaginary part of the polarizability is

$$\Im\left[\frac{1}{k^2\alpha}\right] = -\frac{k}{6\pi}. \tag{S18}$$

Therefore, for non-diffracting gratings at normal incidence

$$\Im\left[\frac{1}{\alpha_y} - G_{byy} + G_{yy}^{(1-2)}\right] = 0, \tag{S19}$$

where we have defined

$$\frac{2}{\alpha_y} = \frac{1}{k^2}\left(\frac{1}{\alpha_y^{(1)}} + \frac{1}{\alpha_y^{(2)}}\right). \tag{S20}$$

The result given by Eq. (S19) is independent of the lattice parameters a, b, d_x and d_y as long as there are no diffraction orders

$$k < min\left(\frac{2\pi}{a}, \frac{2\pi}{b}\right) \quad \leftrightarrow \quad \Im\left[k_{zlp}\right] = 0. \tag{S21}$$