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Supplemental material for Enhanced chirality in dielectric metasurface without breaking symmetry

Xingguang Liu[a,b], Junqing Li*[a], Rui Zhao[a], Yingjie Zhang[a], and Yongkang Dong[c]

1 Physical description of the electromagnetic multipoles and the scattering cross section

It is well known that the physics of an electric dipole (ED) results from positive and negative charges positioned over a distance, whereas a magnetic dipole (MD) is associated with electric current circulating along a closed loop. The higher-order electric and magnetic multipoles, such as electric quadrupoles (EQ), magnetic quadrupoles (MQ) and electric octupoles (EO) should be taken into consideration too. The toroidal dipole (TD) is created by poloidal electric currents flowing on the surface of a torus along its meridians, which can be represented as a set of magnetic dipoles arranged head-to-tail to form a closed loop. The corresponding moments can be expressed as:

$$
\begin{aligned}
\mathbf{P} &= \frac{1}{i\omega}\int \mathbf{J}\ d^3\mathbf{r}\ \text{(ED)},\\
\mathbf{m} &= \frac{1}{2c}\int (\mathbf{r}\times\mathbf{J})\ d^3\mathbf{r}\ \text{(MD)},\\
\mathbf{T} &= \frac{1}{10c}\int [(\mathbf{r}\cdot\mathbf{J})\mathbf{r}-2r^2\mathbf{J}]\ d^3\mathbf{r}\ \text{(TD)},\\
Q_{\alpha\beta} &= \frac{1}{i\omega}\int [r_\alpha J_\beta + r_\beta J_\alpha - \frac{2}{3}(\mathbf{r}\cdot\mathbf{J}\delta_{\alpha\beta})]\ d^3\mathbf{r}\ \text{(EQ)},\\
M_{\alpha\beta} &= \frac{1}{3c}\int [(\mathbf{r}\times\mathbf{J})_\alpha r_\beta + (\mathbf{r}\times\mathbf{J})_\beta r_\alpha]\ d^3\mathbf{r}\ \text{(MQ)},\\
O_{\beta\gamma\tau} &= O'_{\beta\gamma\tau} - (\delta_{\beta\gamma}V_\tau + \delta_{\beta\tau}V_\gamma + \delta_{\gamma\tau}V_\beta)\ \text{(EO)},
\end{aligned} \tag{1}
$$

where $\hat{O}' = -\int \mathbf{prr}+\mathbf{rpr}+\mathbf{rrp}\ d^3\mathbf{r}, \mathbf{V} = \frac{1}{5}\int \mathbf{2}(\mathbf{r}\cdot\mathbf{p})\mathbf{r}+\mathbf{r^2p}\ d^3\mathbf{r}$. c represents the speed of light in vacuum, and α,β,γ,τ stand for Cartesian coordinate x,y,z. $\mathbf{J}$ and $\mathbf{p}$ denote the displacement current density and the electric dipole. $\mathbf{r}$ is the position vector.

The relative strength of the induced dipole and multipole moments contributing to the far-field response of metamaterials can be evaluated based on the general expression of scattering cross section[1]:

$$
\begin{aligned}
\sigma_{\text{sca}} = &\frac{k_0^4}{6\pi\varepsilon_0^2|\mathbf{E}_{\text{inc}}|^2}\left|\mathbf{P}+\frac{ik_d}{v_d}\mathbf{T}\right|^2 + \frac{k_0^4\varepsilon_d\mu_0}{6\pi\varepsilon_0|\mathbf{E}_{\text{inc}}|^2}|\mathbf{m}|^2\\
&+\frac{k_0^6\varepsilon_d}{720\pi\varepsilon_0^2|\mathbf{E}_{\text{inc}}|^2}\left|\sum_{\alpha\beta}Q_{\alpha\beta}\right|^2 + \frac{k_0^6\varepsilon_d^2\mu_0}{80\pi\varepsilon_0|\mathbf{E}_{\text{inc}}|^2}\left|\sum_{\alpha\beta}M_{\alpha\beta}\right|^2,\\
&+\frac{k_0^8\varepsilon_d^2}{1890\pi\varepsilon_0^2|\mathbf{E}_{\text{inc}}|^2}\left|\sum_{\alpha\beta\gamma}O_{\alpha\beta\gamma}\right|^2
\end{aligned} \tag{2}
$$

where $v_d = c/\sqrt{\varepsilon_d}$ and k_d is the speed of light and wave vector in the surrounding medium, respectively. ε_d is the permittivity of the surrounding medium. $|\mathbf{E}_{\text{inc}}|^2$ denotes the intensity of the incident light.

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[a] *Xidazhi Street NO.29, Harbin, China.*

[*] *Junqing Li. E-mail: jqli@hit.edu.cn*

2 The influences of tuning geometric parameters on the BICs

The accidental BIC arises due to the continuous tuning of parameters. Finely tuning the geometric parameters including dx, p, R or s could make the metasurface match the destructive interference condition. Generally speaking, the BICs rely on these geometric characteristics of the metasurface. Let us consider dx, p and R first. When two of them are fixed, tuning the other one can help us find the BICs. To show this clearer, we calculate the transmittance distributions as a function of λ and spacing dx / radius R / period p as shown in Fig. S1. We can find that the BICs can be excited by tuning dx / R / p when the other two are given. And the spectral position of the BICs can be tuned by the width of the gaps s. Fig. S2 gives the transmittance distributions for s spanning from 20 nm to 90 nm. It is clearly seen that a bigger s corresponds to a shorter resonant wavelength.

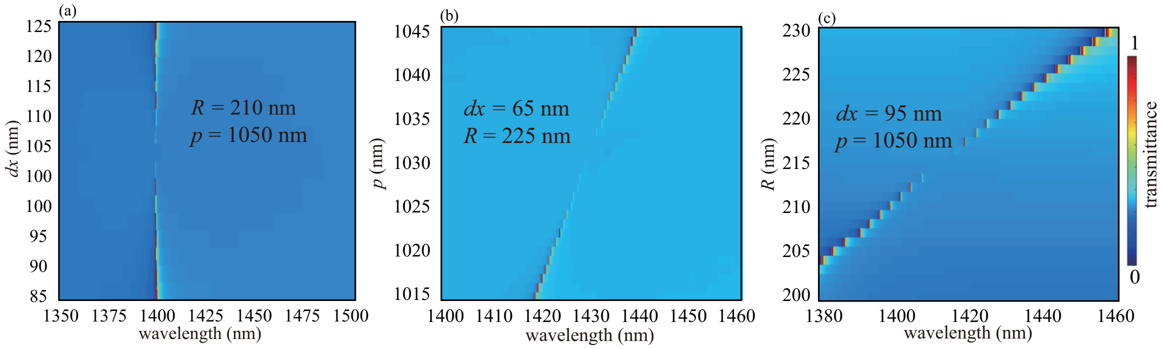

Fig. S1 Transmittance distributions of the metasurface as a function of wavelength λ and (a) spacing dx, (b) period p, (c) radius R of the metasurface.

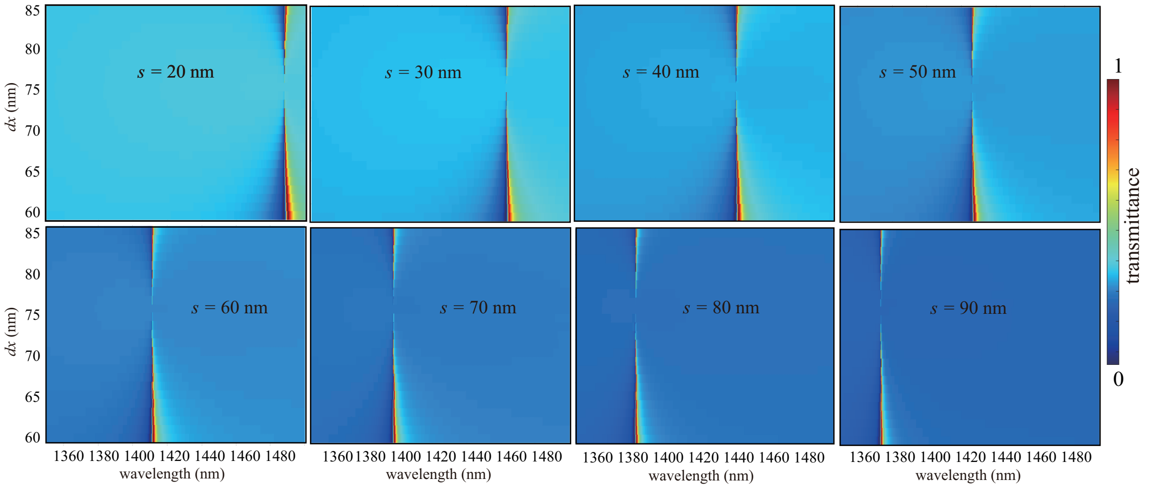

Fig. S2 Transmittance distributions of the metasurface as a function of wavelength λ and dx for different width of the gaps s.

3 The anapole excited on the metasurface

For our metasurface, the TD and ED contributions to the far-field scattering are equal around $\lambda = 1441.1$ nm (Fig. S3(a)) . Moreover, they are out-of-phase (Fig. S3(b)) so that the phase condition $(P = -ik_d T/v_d)$ is fulfilled. As a consequence, the intrinsic anapole state is generated due to the destructive interference of TD and ED modes.

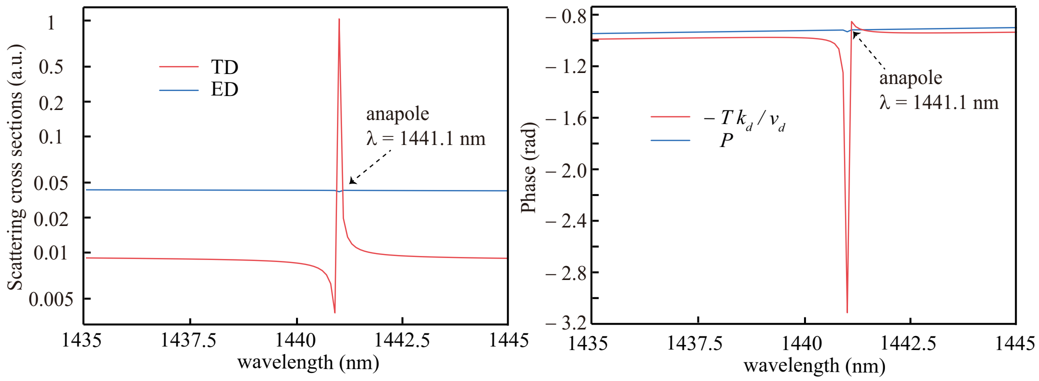

Fig. S3 (a) The multipolar decomposition (ED and TD) scattering cross sections of the metasurface. (b) Phase of the ED and TD moments.

4 The CD of the metasurface with varying chirality

The CD of the metasurface with varying chirality are shown in Fig. S2. It is obviously that bigger chirality can bring larger CD. The chirality of $\kappa = 5\times10^{-2}$ is intentionally chosen to be unphysically large so that we can clear see the CD enhancement.

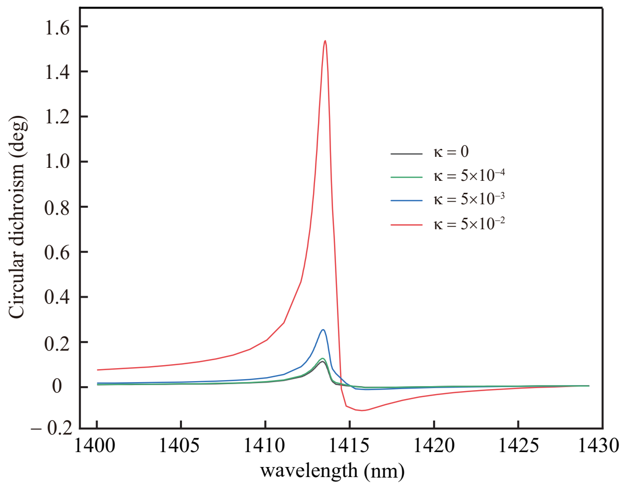

Fig. S4 The CD response of the metasurface for $\kappa = 0$ (black curve), $\kappa = 5\times10^{-4}$ (green curve), $\kappa = 5\times10^{-3}$ (blue curve) and $\kappa = 5\times10^{-2}$ (red curve).

5 The anapole excited on the metasurface

In Fig. S5, we give the simulated CD for the metasurface if the chiral analyte is not sit at the slits (the red curve). We can find that, the CD only have a small changes in the amplitude and spectral position compared with the CD if the chiral analyte can sit at the slits. Therefore, there is only a little influence on the chirality enhancement effect even if the analyte on top of the metasurface is not sit exactly at the optimal positions (slits)

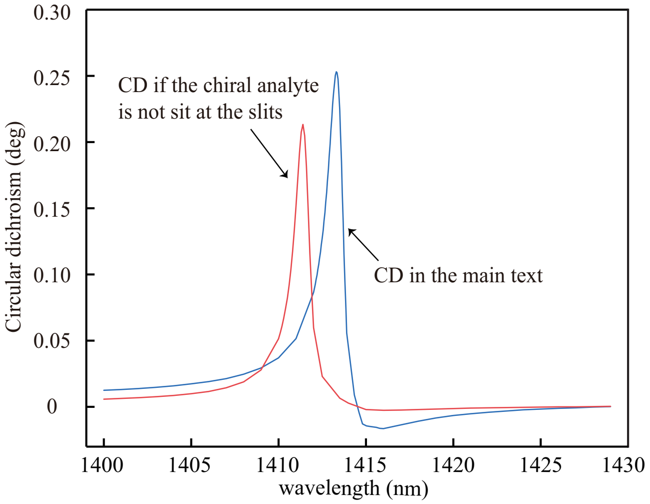

Fig. S5 CD responses of the metasurface if the chiral analyte is not sit at the slits (red curve). CD of the metasurface if the chiral analyte can sit at the slits (blue curve).

References

1 A. B. Evlyukhin, T. Fischer, C. Reinhardt and B. N. Chichkov, *Physical Review B*, 2016, **94**, 205434.