Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Multifunctional terahertz metasurfaces for polarization transformation and wavefront manipulation

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S1: Derivation of Jones matrix

The polarization state of monochromatic polarized plane light can be described by a complex vector: $\mathbf{E}=\begin{bmatrix}E_x\\E_y\end{bmatrix}$. The polarization dependent devices can be described by Jones matrix T. The polarization state of the output beam can be obtained by multiplying the Jones vector of the input light by the Jones matrix of the device: $\mathbf{E}_{out}=T\mathbf{E}_{in}$.

The PB device, for example, is typically a special kind of half-wave plate. It is assumed that the fast axis of the half wave plate is in the x direction and the slow axis is in the y direction. Then the Jones matrix of the half wave plate can be written as: $T=\begin{bmatrix}1&0\\0&1\end{bmatrix}$.

Half wave plate is usually used to rotate the polarization state of linearly polarized light. As shown in Fig. S1, considering that the coordinates (vectors) in the large XY coordinate system need to be represented by the coordinates in the small xy coordinate system, the coordinate transformation is given by the following equation:

$$\begin{aligned}X&=x\cos\alpha-y\sin\alpha\\Y&=x\sin\alpha+y\cos\alpha\end{aligned}$$ * MERGEFORMAT (S1).

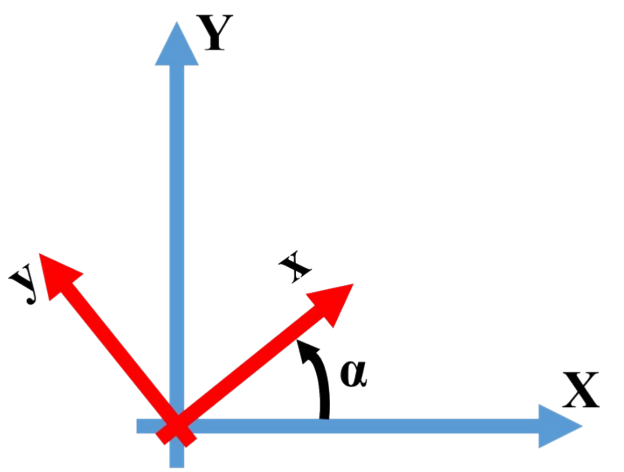


Fig. S1 Transformation image of coordinate system

Write Equation (S1) in matrix form:

$$\begin{bmatrix}X\\Y\end{bmatrix}=R\begin{bmatrix}x\\y\end{bmatrix}=\begin{bmatrix}\cos\alpha&-\sin\alpha\\\sin\alpha&\cos\alpha\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix}$$ * MERGEFORMAT (S2),

where R is the rotation matrix. The Jones matrix of the previous half wave plate assumes that the fast axis of the half wave plate is in the x direction and the slow axis is in the y direction. However, if it is necessary to simulate a half wave plate rotated by a certain angle, this rotation matrix can be used. We can define a coordinate system for fast axis and slow axis, which is called component coordinate system. Component coordinate system is represented by lowercase xy. In this coordinate system, its input and output can be expressed by the following equation:

$$\begin{bmatrix}E_x\\E_y\end{bmatrix}_{out}=T\begin{bmatrix}E_x\\E_y\end{bmatrix}_{in}$$ * MERGEFORMAT (S3),

where *T* is the Jones matrix in the component coordinate system. Then the horizontal and vertical directions of the laboratory define a coordinate system, which is called the laboratory coordinate system. It is represented by the uppercase XY. Then, the representation of the Jones vector of polarized light in these two coordinates systems is given by the corresponding lowercase and uppercase subscripts. Simultaneously, it is assumed that there is only rotation relationship between the two coordinate systems, then there is:

$$\begin{bmatrix} E_X \\ E_Y \end{bmatrix} = R \begin{bmatrix} E_x \\ E_y \end{bmatrix}$$ * MERGEFORMAT (S4).

The identity matrix acts on both sides of the Equation (S3) at the same time:

$$R^{-1}R\begin{bmatrix} E_x \\ E_y \end{bmatrix}_{out} = TR^{-1}R\begin{bmatrix} E_x \\ E_y \end{bmatrix}_{in}$$ * MERGEFORMAT (S5).

Substituting Equation (S4) into Equation (S5), we can get:

$$R^{-1}\begin{bmatrix} E_X \\ E_Y \end{bmatrix}_{out} = TR^{-1}\begin{bmatrix} E_X \\ E_Y \end{bmatrix}_{in}$$ * MERGEFORMAT (S6).

Apply the rotation matrix to Equation (S6):

$$\begin{bmatrix} E_X \\ E_Y \end{bmatrix}_{out} = RTR^{-1}\begin{bmatrix} E_X \\ E_Y \end{bmatrix}_{in}$$ * MERGEFORMAT (S7).

According to the above two relations, the Jones matrix in the laboratory coordinate system can be written as:

$$T_\alpha = RTR^{-1}$$ * MERGEFORMAT (S8).

S2: Derivation of Jones matrix for polarization conversion from linear polarization to circular polarization

For the rectangular silicon cylinder whose length and width are parallel to the x-axis or y-axis, there is no cross-polarization component when x-LP or y-LP wave is incident. Similarly, for a silicon elliptical pillar with its major axis on the x-axis or y-axis, under x-LP or y-LP incidence, only the components with the same incident polarization are transmitted. Therefore, the transfer matrix T can be expressed as:

$$T = \begin{bmatrix} t_{xx}e^{i\varphi_x} & 0 \\ 0 & t_{yy}e^{i\varphi_y} \end{bmatrix}$$ * MERGEFORMAT (S9),

where t_{xx} and φ_x represent the amplitude and phase of x-LP component of exit wave respectively, and t_{yy} and φ_y represent the amplitude and phase of y-LP component respectively. According to **S1**, a new Jones matrix T_α is formed when the rotation angles of a silicon rectangular cylinder or elliptical cylinder are α to the x-axis:

$$T_\alpha = RTR^{-1} = \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix}\begin{bmatrix} t_{xx}e^{i\varphi_x} & 0 \\ 0 & t_{yy}e^{i\varphi_y} \end{bmatrix}\begin{bmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{bmatrix}$$ * MERGEFORMAT (S10).

Furthermore, we consider the incident x-LP wave, that is $|\mathbf{H}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\mathbf{E}_{out1}$ of the exit wave is:

$$\mathbf{E}_{out1} = T_\alpha|\mathbf{H}\rangle = \begin{bmatrix} t_{xx}e^{i\varphi_x}\cdot\cos^2\alpha + t_{yy}e^{i\varphi_y}\sin^2\alpha \\ t_{xx}e^{i\varphi_x}\cdot\sin\alpha\cos\alpha - t_{yy}e^{i\varphi_y}\sin\alpha\cos\alpha \end{bmatrix}$$ * MERGEFORMAT (S11),

when the following conditions are satisfied: $t_{xx} = t_{yy}$, $\alpha = \pi/4$, $\varphi_y = \varphi_x + \pi/2$, Equation (S11) can be expressed as:

$$\mathbf{E}_{out1} = \frac{t_{xx}e^{i\varphi_x}}{2}\begin{bmatrix} 1+i \\ 1-i \end{bmatrix} = \frac{\sqrt{2}}{2}t_{xx}e^{i(\varphi_x+\pi/4)}\begin{bmatrix} 1 \\ -i \end{bmatrix} = m|\mathbf{L}\rangle$$ * MERGEFORMAT (S12).

Similarly, under y-LP incidence, that is $|\mathbf{V}\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $\vec{E}_{out1}$ of exit wave will be expressed as:

$$\begin{aligned}\mathbf{E}_{out1} &= \begin{bmatrix} t_{xx}e^{i\varphi_x}\cdot\sin\alpha\cos\alpha - t_{yy}e^{i\varphi_y}\sin\alpha\cos\alpha \\ t_{xx}e^{i\varphi_x}\cdot\sin^2\alpha + t_{yy}e^{i\varphi_y}\cos^2\alpha \end{bmatrix} \\ &= \frac{\sqrt{2}}{2}t_{xx}e^{i(\varphi_x-\pi/4)}\begin{bmatrix} 1 \\ i \end{bmatrix} = m_1|\mathbf{R}\rangle\end{aligned}$$ * MERGEFORMAT (S13).

S3: Derivation of Jones matrix for polarization conversion from circular polarization to linear polarization

In **S2**, when $t_{xx} = t_{yy}$, $\alpha = \pi/4$, $\varphi_y = \varphi_x + \pi/2$, Equation (S10) can also be simplified as:

$$T_\alpha = \frac{\sqrt{2}}{2}t_{xx}e^{i\varphi_x}\begin{bmatrix} e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}} \\ e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}} \end{bmatrix}$$ * MERGEFORMAT (S14).

Under the RCP incidence, the electric field $\vec{E}_{out2}$ of output beam can be expressed as:

$$\mathbf{E}_{out2} = T_\alpha|\mathbf{R}\rangle = \frac{\sqrt{2}}{2}t_{xx}e^{i\varphi_x}\begin{bmatrix} e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}} \\ e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}} \end{bmatrix}\begin{bmatrix} 1 \\ i \end{bmatrix} = \sqrt{2}t_{xx}e^{i(\varphi_x+\pi/4)}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = n|\mathbf{H}\rangle$$ * MERGEFORMAT

Considering the incident LCP wave, then the electric field $\vec{E}_{out2}$ of output beam is:

$$\mathbf{E}_{out2} = T_\alpha|\mathbf{L}\rangle = \frac{\sqrt{2}}{2}t_{xx}e^{i\varphi_x}\begin{bmatrix} e^{i\frac{\pi}{4}} & e^{-i\frac{\pi}{4}} \\ e^{-i\frac{\pi}{4}} & e^{i\frac{\pi}{4}} \end{bmatrix}\begin{bmatrix} 1 \\ -i \end{bmatrix} = \sqrt{2}t_{xx}e^{i(\varphi_x-\pi/4)}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = n_1|\mathbf{V}\rangle$$ * MERGEFORMA

S4: Select the meta-atom to realize the

polarization conversion from x-linear polarization to left-hand circular polarization

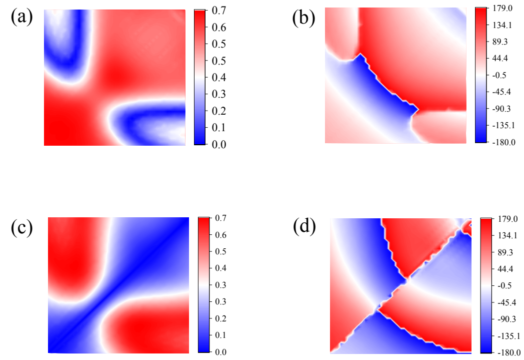


Fig. S2 Characterization of meta-atoms with rectangular pillar structure. (a-b) Simulated amplitudes and phase shifts of the x-polarized component at the transmission end under x-LP incidence at 1 THz. (c-d) Simulated transmission amplitudes and phase shifts of the y-polarized component under x-LP incidence at 1 THz.

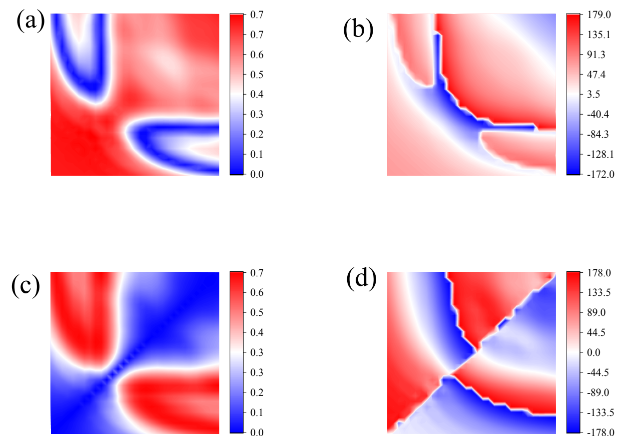
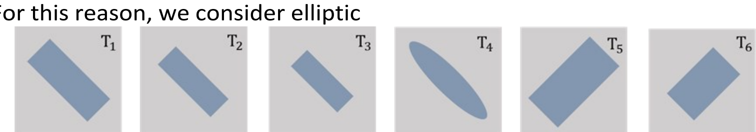


Fig. S3 Characterization of meta-atoms with elliptic pillar structure. (a-b) Simulated transmission amplitudes and phase shifts of the x-polarized component under x-LP incidence at 1 THz respectively. (c-d) Simulated amplitudes and phase shifts of the y-polarized component at the transmission end under x-LP incidence at 1 THz respectively.

In this paper, the time domain solver of CST Microwave Studio is used to scan the parameters. We set the length and width of the rectangular pillar in the interval 30 - 110, and calculate the length in μm with the step size of 2. We derive the simulation results to calculate the amplitude and phase of x-LP and y-LP waves respectively, as shown in Fig. S2. Obviously, when the amplitude of y-LP wave is equal to that of x-LP wave, and the phase difference is close to 90° for a single rectangular pillar structure, a phase variation of 2π cannot be achieved by this structure. For this reason, we consider elliptic pillar structure. Set the major axis and minor axis of the elliptical pillar within 10 - 60 and calculate in steps of 1, with the length unit of μm. The final calculation result is shown in Fig. S3. In a word, neither of the two structures can achieve a phase variation of 2π under the condition of polarization conversion from linear polarization to circular polarization. After comparative analysis, six meta-atoms chosen from the two structures are considered, and the specific parameters are given in Fig. S4.



	T_1	T_2	T_3	T_4	T_5	T_6
D_1	56	52	45	20	61	59
D_2	72	66	64	108	120	85

Fig. S4 The structure image and corresponding specific parameters of the six selected meta-atoms.

S5: Select the meta-atom to realize the polarization conversion from x-linear polarization to right-hand circular polarization

As shown in Fig. S5(a), in order to realize the polarization conversion from x-linear polarization to right-hand circular polarization, we introduce the mirror symmetrical structure of the above six meta-atoms in Fig. S4. Fig. S5 (b) illustrates the transmission ratio t_{yx}/t_{xx} of the simulated six meta-atoms, and Fig. S5 (c) shows the phase difference $\Delta\varphi$ between the y and x components of exit wave under x-LP incidence at 1 THz. The six kinds of mirror symmetrical meta-atoms have specific functions: when x-LP wave is incident, the amplitude ratio of transmitted terahertz wave in y direction and x direction is close to 1, and the phase difference $\Delta\varphi$ in these two directions is close to 90°, which means that exit wave is RCP.

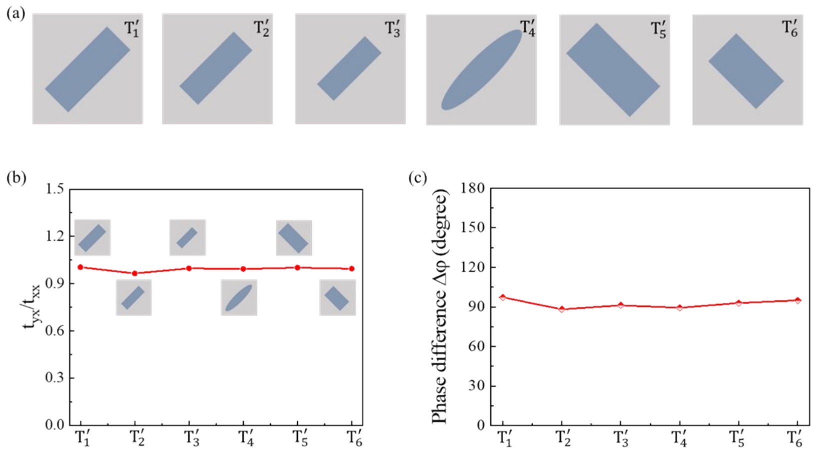


Fig. S5 (a) Schematic the mirror structure corresponding to the six meta-atoms in Fig. S4 and each structure operates at 1THz. (b) The simulated transmission ratio of the y component and the x component of six meta-atoms in (a). (c) Simulated the phase difference between the y and x components of six meta-atoms in (a) under x-LP incidence.

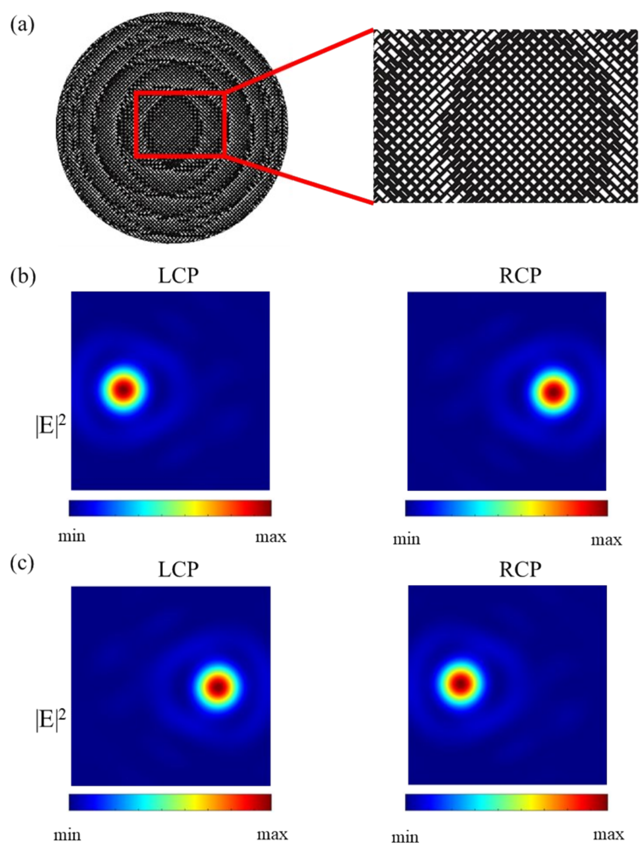


Fig. S6 (a) The structure image of the designed metasurface. (b) The simulative and experimental results for focusing and conversion of incident x-linear to transmission circular polarization. (c) The electric field distribution of LCP and RCP waves on the focal plane under the y-LP illumination.

S6: Design of bifocal metasurface

Based on the phase arrangement in the text, we design a bifocal metasurface, whose structure is shown in Fig. S6(a). For example, under the x-LP incidence, two polarization focuses with opposite spin directions are generated in the focal plane. Based on the Equation (5) in the main body of the paper, the following conditions are satisfied when arranging the phase of the meta-atoms realizing polarization conversion from x-linear polarization to left-hand circular polarization: λ = 300 μm, x_1 = -450 μm, y_1 = 0 μm, f = 7 mm. For the above-mentioned meta-atoms, the phase arrangement of the mirror structure also meets the Equation (5) in the main body of the paper, and the specific parameters are: λ = 300 μm, x_1 = -450 μm, y_1 = 75 μm, f = 7 mm. The simulated and experimental results for focusing and conversion of incident LP wave to transmission CP wave are shown in Figs. S6(b) and S6(c), respectively. In addition, combined with **S3**, under the CP incidence, two orthogonal LP beams are generated and focused on different positions. In a word, the metasurface realizes the bidirectional polarization conversion between linear polarization and circular polarization, and simultaneously generates two different focal points in space.