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Chiral Quasi-Bound States in the Continuum

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Quasi-bound states in the continuum (q-BICs) are Fano resonant states with long optical lifetimes controlled by symmetry-breaking perturbations. While conventional Fano responses are limited to linear polarizations and do not support tailored phase control, here we introduce q-BICs born of chiral perturbations that encode arbitrary elliptical polarization states and enable geometric phase engineering. We thereby design metasurfaces with ultrasharp spectral features that shape the impinging wavefront with near-unity efficiency. Our findings extend Fano resonances beyond their conventional limits, opening opportunities for nanophotonics, classical and quantum optics, and acoustics.

Suitably designed photonic crystal slabs (PCSs) have been recently shown to support quasi-bound states in the continuum (q-BICs): Fano resonant modes whose radiative lifetime is controlled by symmetry-lowering perturbations [1] that become non-radiating states [2]-[4] due to symmetry-protection in the absence of the perturbation. When light with a polarization state matching the q-BIC eigenpolarization impinges on the structure, an ultrasharp Fano response arises [5], and the resonantly scattered light maintains the same polarization. This property, combined with strong in-plane Bragg scattering in high-contrast index systems [6], enables compact optical devices concentrating light in both space and time [7]-[11]. By perturbing every other unit cell in such

systems, the Brillouin zone folds, enabling access to previously bound modes and providing additional design freedom to control q-BICs in real- and momentum-space [10]-[13]. Photonic crystals supporting q-BICs hence offer a highly versatile platform for biological sensing [14], planar optical modulators [15], notch filters [16] and nonlinear optics [17],[18].

Recently, the selection rules for q-BICs in planar photonic crystals have been classified, clarifying to which (if any) free-space polarization state a q-BIC couples due to a chosen symmetry perturbation [13]. This result implies that the q-BIC polarization must be linear in planar structures that preserve symmetry across a horizontal plane. Adiabatically varying this polarization angle in the lateral direction introduces a spatially varying geometric phase, enabling metasurface functionalities such as anomalous reflection and refraction for circularly polarized light [13]. However, due to the planarized symmetry and the linear polarization constraint, the maximum achievable efficiency of wavefront shaping is 25% [19].

Breaking this symmetry with the introduction of optical chirality may enable devices with strong circular dichroism [22]-[29]. A common approach to achieve strong optical chirality is the spectral superposition of two modes supported by structures with intrinsic geometrical asymmetries [30],[31]. Recent work has demonstrated metasurfaces that vary the geometric phase associated with spin-preserving chiral structures in devices with asymmetric transmission profiles [32]-[34]. In parallel, the emerging field of twistronics has been exploring how anisotropic parallel layers stacked with a twist with respect to one another can exhibit unexpected electronic [35] and optical [36],[37] properties pertaining to the eigenstates of the composite system, opening new degrees of freedom in engineering wave-matter interactions.

Motivated by these recent advances, in this Letter we show that a pair of tightly stacked interfaces, each with a distinct perturbation, can support Fano resonances born of chiral q-BICs: spectrally isolated, non-degenerate modes whose coupling to free-space is intrinsically chiral. As in other q-BIC systems, the perturbation weakly alters the mode so that it leaks to free-space with a scattering rate determined by the magnitude of the perturbation and to a polarization state determined by symmetry (i.e., governed by selection rules). Unlike conventional q-BICs however, which are limited to linear polarizations and a fixed phase response, we show that this polarization state can be arbitrarily elliptical with any desired phase at resonance. The resulting Fano resonances exhibit designer elliptical dichroism, engineerable with complete and continuous coverage of the Poincare sphere. In particular, circularly polarized light may be selected with any in-plane orientation, resulting in a spin-selective Fano resonance encoding arbitrary geometric phase. Our finding enables Fano resonant metasurfaces that can shape an impinging wavefront with near-unity efficiency (spin selectivity) exclusively across a designer bandwidth of choice (spectral selectivity). Since these concepts originate solely from symmetry perturbations, we anticipate their extension to other physical domains supporting Fano resonances, such as at radio-frequencies or in acoustics.

Consider a slab supporting a symmetry-protected BIC controlled by two homogenized interfaces, engineered to scatter the trapped energy to the far field by breaking a relevant symmetry. We assume that the bottom and top interfaces scatter light to linear polarization states oriented at angles ϕ_1 and ϕ_2 , respectively, where in the achiral case $\phi_1 = \phi_2$ due to symmetry, while in the general chiral case [Fig.1(a)] ϕ_1 and ϕ_2 are different. Based on temporal coupled mode theory (TCMT) [38],[39], we can write the states leaking upwards and downwards respectively as:

$$\begin{aligned}
|e_u\rangle &= \frac{1}{\sqrt{\tau}} \left\{ \mp \begin{bmatrix} \cos(\phi_1) \\ \sin(\phi_1) \end{bmatrix} + i \begin{bmatrix} \cos(\phi_2) \\ \sin(\phi_2) \end{bmatrix} \right\} \\
|e_d\rangle &= \frac{1}{\sqrt{\tau}} \left\{ i \begin{bmatrix} \cos(\phi_1) \\ \sin(\phi_1) \end{bmatrix} \mp \begin{bmatrix} \cos(\phi_2) \\ \sin(\phi_2) \end{bmatrix} \right\},
\end{aligned} \tag{1}$$

where τ is the optical lifetime of the mode controlled through the magnitude of the symmetry perturbation, the top (bottom) sign corresponds to the symmetric (antisymmetric) mode in the z direction, and the factor i accounts for the relative scattering phase of the top and bottom interfaces [38].

Such metasurfaces may be implemented with properly chosen perturbations applied to otherwise high-symmetry PCSs: in Fig. 1(b) an unperturbed periodic permittivity profile H^0 (circular holes etched in a high index slab) is successively perturbed into structures V_1 at the bottom interface (two ellipses oriented at α and $\alpha + 90^\circ$) and V_2 at the top interface (two ellipses oriented at $\alpha + \Delta\alpha$ and $\alpha + \Delta\alpha + 90^\circ$). The period in one direction is doubled from a to $2a$ due to this perturbation, allowing excitation of modes that were previously guided [11]. When $\Delta\alpha$ is properly chosen so that $\phi_2 = \phi_1 \pm \pi/2$, the leaking states are right-handed circularly polarized (RCP). Hence, upon excitation by a plane wave at normal incidence (either from below or above) the device shows full circular dichroism: RCP light is resonantly reflected and left-handed circularly polarized (LCP) light is non-resonantly transmitted [Fig. 1(c)].

Both spectral selectivity (linewidth) and spin selectivity (handedness) of the optical response originate from and are controllable through the symmetry perturbation. To demonstrate this, Figs. 1(d,e) show three-dimensional schematics of the unperturbed and perturbed geometry [whose spectra are shown in Fig. 1(c), calculated by finite difference time domain simulations (Lumerical

Solutions)]. Here, a thin Si film of height $h = 1.25a$ and refractive index $n = 3.45$ is suspended in SiO_2 , with refractive index $n_0 = 1.45$, filling circular inclusions with diameter D_0 [Fig. 1(d)] or elliptical inclusions [Fig. 1(e)] with diameters $D_0 \pm \delta/2$ (δ quantifies the magnitude of the perturbation). We note that such a structure may be manufactured by multi-step lithography and planarization at telecommunications wavelengths [40],[41]. The quasi-TE mode supported by the unperturbed structure is bound to the slab [Fig. 1(f)] and it is characterized by a vertically antisymmetric out-of-plane magnetic field H_z [corresponding to the bottom sign in Eq. (1)]. Upon perturbation [Fig. 1(g)], the H_z profile is weakly perturbed such that an induced chiral moment scatters light upwards and downwards as RCP waves (demonstrated by the quantities $H_x \pm iH_y$, where the complex conjugation reflects a change in direction, not handedness). The device in Fig. 1(e) thereby supports a chiral q-BIC: a long-lived optical state that, by construction, has a Q-factor varying as $Q \propto 1/\delta^2$ [1] and selection rules that are intrinsically chiral, leaking exclusively to a single circular polarization channel.

In particular, the selection rules of each interface prescribe coupling to light polarized at angles ϕ_1 (following $\phi_1 \approx 2\alpha$) for V_1 , and ϕ_2 (following $\phi_2 \approx 2(\alpha + \Delta\alpha)$) for V_2 [13],[38]. Upon insertion into Eqn. (1), this implies that the orientation angles of the real and imaginary parts of the scattered light are separately and arbitrarily controlled, and hence elliptical dichroism is possible. This is shown in Fig. 2 by varying $\Delta\alpha$ from -90° to 90° and α from 0° to 90° , and studying the eigenpolarizations of the corresponding q-BICs by analyzing the Jones matrix for the transmitted light at the resonant frequency. As an example, Fig. 2(a) maps the peak reflectance R for the metasurface of Fig. 1(e) with $\alpha = 47^\circ$ and $\Delta\alpha = 31^\circ$ as a function of the ellipticity parameters of

the polarization state 2χ and 2ψ , representing the latitude and longitude on the Poincare sphere, respectively. We find a peak with near-unity reflectance (marked with a red dot) and with near-unity transmittance (marked with a blue dot) at the resonant frequency. Figure 2(b) shows the reflectance spectra for these two extremal cases, demonstrating a Fano resonance for one of the eigenpolarizations, and minimal response for the orthogonal state. The inset shows that the eigenpolarization maintains its polarization state, including its handedness, upon reflection. The values of 2χ and 2ψ may be determined for every choice of $\Delta\alpha$ and α using a similar procedure, and are shown in Figs. 2(c,d). Hence, by varying the metasurface geometry we can span the Poincare sphere, with 2χ controlled by $\Delta\alpha$ and 2ψ controlled by both α and $\Delta\alpha$ [38].

Next, we study metasurfaces designed for RCP illumination where the elliptical eigenpolarization is spatially varied across the device. We begin by building a library of meta-units (the building blocks of a spatially varying metasurface) capable of controlling both the amplitude and phase of the resonantly reflected RCP light, comparable to the results in Ref. [43] but applied only across the designed bandwidth of the q-BIC. For RCP light incident on a device with eigenpolarization $|e\rangle$, the complex amplitude of the RCP component of the reflected wave is

$$E_R = \langle e|R \rangle^2 = \frac{1}{2}(1 + \sin(2\chi))e^{2i\psi}. \quad (2)$$

The remaining states (LCP in reflection, LCP and RCP in transmission) may be easily written as well [38]. The amplitude of reflected RCP light therefore varies from 0 to 1 as 2χ varies from $-\pi/2$ to $\pi/2$ (the poles of the Poincare sphere) while the phase is $\Phi = 2\psi$. According to the relation between 2ψ and α in Fig. 2(d), the phase of the reflected RCP light varies as $\Phi \sim 4\alpha$.

Full-wave simulations (Lumerical Solutions) confirm this picture: Fig. 3(a) shows how the spectral reflectance for RCP light can arbitrarily vary between zero and unity by simply changing $\Delta\alpha$, and Fig. 3(b) shows that the spectral phase function can be substantially controlled to allow any phase value at resonance by varying α , markedly different from a conventional resonant metasurface. Figures 3(c,d) map the amplitude and phase of reflected RCP light as a function of α and $\Delta\alpha$, showing that we can achieve any desired value. In [38] we invert this information to create a look-up table prescribing the geometry that achieves any desired complex reflection coefficient. This tool is ideal to apply the concept of geometric phase to a chiral q-BIC metasurface with slow variations of amplitude and phase in its transverse plane synthesizing arbitrary wavefronts with large efficiency. Compared to conventional Fano resonances and metasurfaces, chiral q-BICs enable highly efficient transformations exclusively across controllable linewidths, while remaining fully transparent for other frequencies.

Figure 4 demonstrates, as an example, a phase-gradient chiral q-BIC metasurface anomalously reflecting incoming RCP light with near-unity efficiency only at resonance (with near-zero efficiency off resonance). We construct a sub-library of Fig. 3 with maximal amplitude and complete phase coverage, seen in Fig. 4(a) [38]. This sub-library provides a spatial phase gradient by varying α ; linearly varying the phase across a superperiod of $16a$ results in a metasurface that generates a tilted planewave with in-plane momentum $k_g = \pm\pi/8a$ [Fig. 4(b)]. Due to this additional momentum imparted during the scattering process, when excited from normal incidence a spatially varying dark mode is observed with a Bloch wavevector k_g [shown overlaid with the geometry in Fig. 4(c)]. This encoded momentum is imparted both upon coupling in and out [19], meaning that the outgoing light is deflected by a total of $2k_g$. The far field for each wavelength is

shown in Figs. 4(d,e) for RCP and LCP light, demonstrating near-unity anomalous reflection when RCP light is incident, and near-unity specular transmission when LCP light is incident.

Notably, despite the presence of nine distinct diffraction orders for each polarization state in both transmission and reflection sides, the metasurface supports a sharp Fano resonance with near-unity reflectance to an arbitrary angle (the $m = \pm 2$ diffraction order). This behavior stands in stark contrast to conventional Fano metasurfaces, wherein additional diffraction orders act as significant loss pathways in the scattering process. The period of the structure is typically made sufficiently subwavelength to support only two diffraction orders [11], avoiding unwanted energy pathways and guaranteeing unity reflectance in the absence of material loss. This discrete translational symmetry is necessarily broken in our system in order to impart the phase gradient and yet, since our system is constructed by weakly perturbing a 0th order grating, it maintains the very large efficiency while offering a designer phase profile that selects which angles are involved in the Fano resonance. Conservation of linear momentum would preclude all but four orders ($m = 0$ and $m = \pm 2$, with the sign determined by the spin) [19], but the resulting achirality results in a system with a maximum of 25% diffraction efficiency that necessarily splits the resonant light into four channels according to the spin [38]. Here, in contrast, spin-selectivity eliminates the pathways corresponding to the non-resonant circular polarization, realizing a true two-port generalized Fano resonance with wavefront-shaping functionality and coupling to a single output channel with near-unity efficiency.

More complex wavefront shaping, such as focusing or orbital angular momentum generation, is generally possible following similar principles. The library in Fig. 3 enables arbitrary phase-amplitude holography encoded in a chiral q-BIC and optically reconstructable only using the correct input polarization and wavelength; all non-resonant wavelengths will see a slab acting as

a weakly perturbed effective medium. In total, a chiral q-BIC enables engineering with large flexibility the Fano resonance Q-factor, resonant wavelength, and phase-amplitude response simultaneously by tuning the magnitude of the perturbation, unperturbed lattice geometry, and orientation angles of the chiral structure, respectively. Notably, unlike recent demonstrations of polarization vortices born of BICs [44],[45], the control of the q-BIC properties is here in real space, rather than in momentum space. As a consequence, spatial variations of the phase-amplitude response directly translate into control of the local diffraction angles and diffraction efficiencies, and are thereby applicable to finite-sized beams with a large spread of momentum [19]. The approach outlined here therefore drastically advances the control of Fano resonances with spatially tailored dark modes, establishing an exciting platform for applications such as augmented reality and secure optical communications, which enable a broadband transparent response unless interrogated in a very narrow spectral range with a specific eigenpolarization of choice.

In conclusion, we have shown that Fano responses are not bound to linear polarizations and specific amplitude and phase response at resonance. By introducing q-BICs based on chiral symmetry perturbations, we have expanded the range of available eigenpolarization states for ultrasharp resonances to the entire Poincare sphere. When the eigenpolarization is circularly polarized, the device supports a Fano resonance exhibiting full circular dichroism, for which the resonant eigenpolarization is reflected and the orthogonal polarization transmitted with near-unity efficiency and arbitrarily sharp frequency selectivity. When the incident light is circularly polarized, varying the eigenpolarization of the device tunes the amplitude and phase of reflected light of the same spin at will, opening totally new opportunities for Fano-based metasurfaces. By applying geometric phase concepts, we are able to realize ultrasharp resonant metasurfaces with arbitrary spatial phase profiles intrinsically encoded in an engineered dark mode with near-unity

amplitude, ideal for highly spectrally and spin selective wavefront shaping. These results are deeply rooted in symmetries, implying that the concepts behind these generalized Fano resonances are not limited to flat optics applications, but can be extended to a wide range of wave-based systems, from acoustics and radio-frequencies to quantum photonics.

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Figures

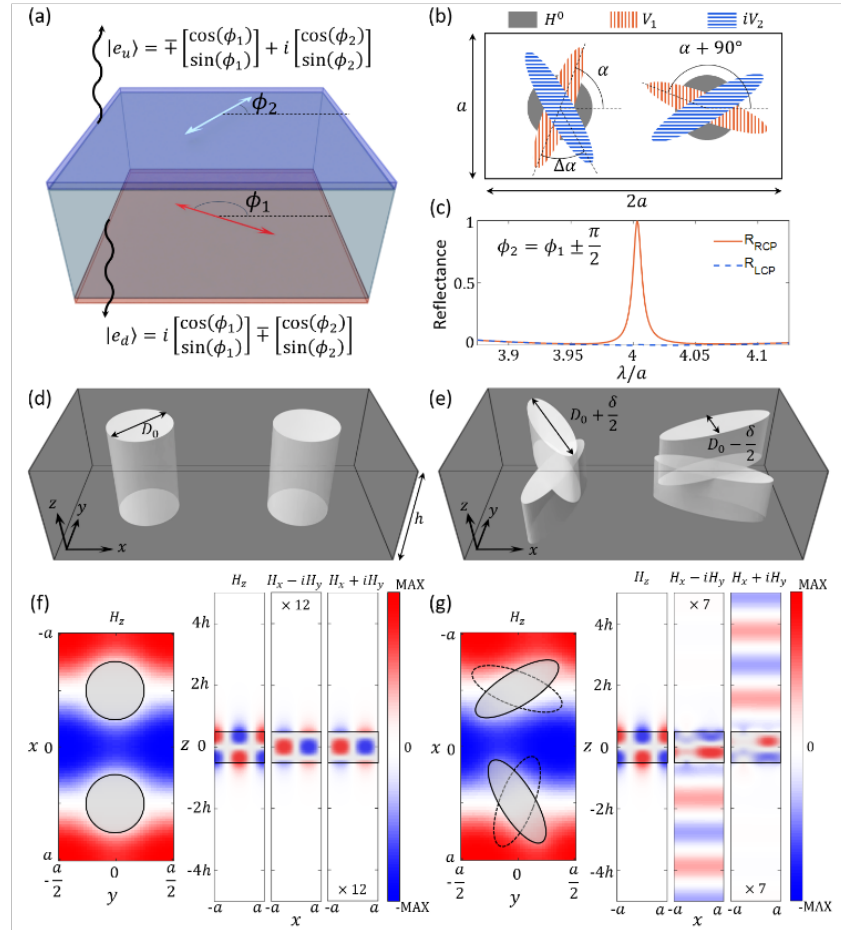


Figure 1. Chiral q-BICs. (a) Homogenized model of a metasurface supporting a chiral q-BIC: two interfaces scatter optical energy to linearly polarized free-space light with polarization angles ϕ_1 and ϕ_2 , respectively, resulting in chiral states leaked upwards and downwards, $|e_u\rangle$ and $|e_d\rangle$. (b) Perturbation scheme involving two perturbations, V_1 and V_2 , for control over ϕ_1 and ϕ_2 , respectively. (c) Example spectra of a device based on the scheme in (b) (with $\alpha = 70^\circ$ and $\Delta\alpha = 50^\circ$) showing full circular dichroism only at resonance. (d,e) Unperturbed and perturbed structures, respectively. (f,g) Unperturbed and perturbed magnetic field components, showing that the bound state (principally characterized by H_z) leaks to RCP light when perturbed.

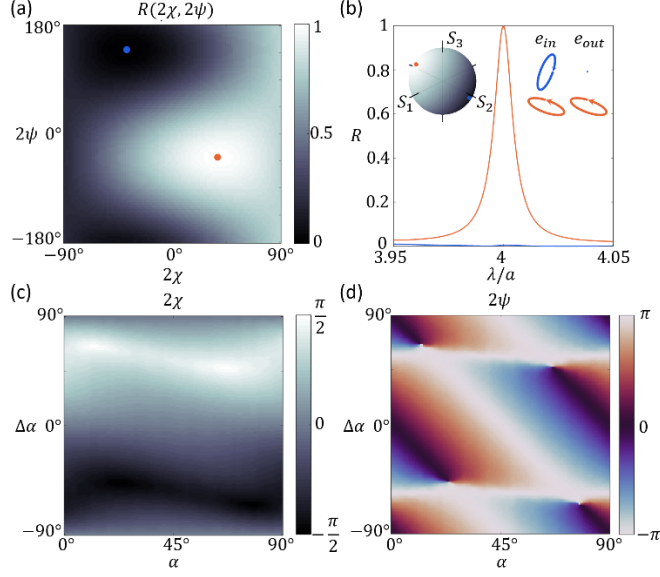


Figure 2. Fano resonances with arbitrary elliptical eigenpolarizations. (a) Map of reflectance for a device with $\alpha = 47^\circ$ and $\Delta\alpha = 31^\circ$ as a function of input polarization state (characterized by the latitude, 2χ , and longitude, 2ψ , on the Poincare sphere). (b) Reflectance spectra for the extremal cases in (a) (marked by red and blue dots), with the insets showing the eigenpolarization states, e , that are maximally and minimally resonant and their positions on the Poincare sphere. (c,d) Map of the coverage of the Poincare sphere for the maximally resonant elliptical eigenpolarization as a function of α and $\Delta\alpha$.

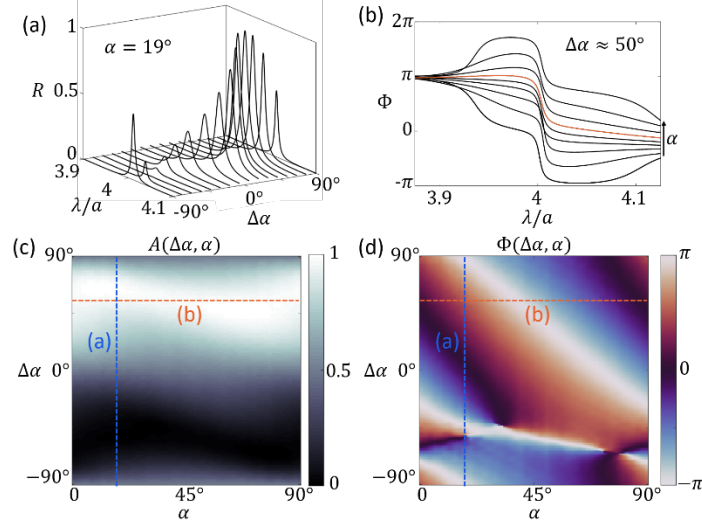


Figure 3. Full control over amplitude and phase of resonantly reflected light. (a) Spectral reflectance near the resonance for $\alpha = 19^\circ$ and sampled values of $\Delta\alpha$. (b) Spectral phase near the resonance for $\Delta\alpha \approx 50^\circ$ and sampled values of α . Orange curve highlights the conventional phase function expected for a Fano resonance. (c,d) Amplitude, A , and phase, Φ at the resonant wavelength for reflected RCP light as a function of α and $\Delta\alpha$, with the contours sampled in (a,b) highlighted.

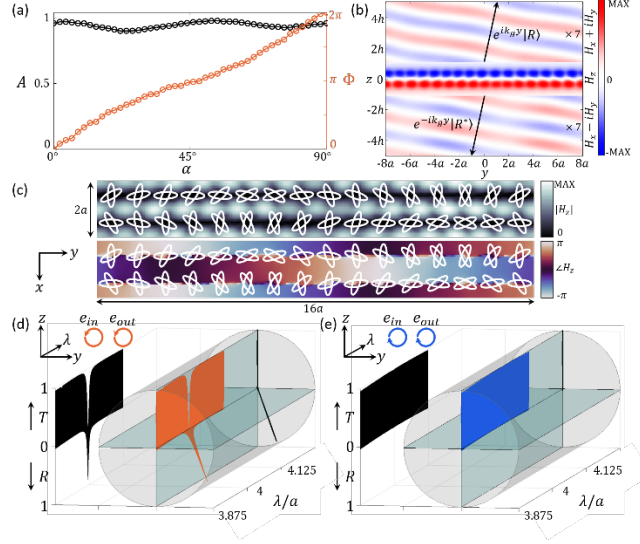


Figure 4. Chiral phase-gradient resonant metasurface with near-unity diffraction efficiency. (a) Sub-library of Fig. 3(c,d) with near-unity amplitude and phase varying over 2π . (b) Device with a spatially tailored leaky mode encoding a coupling phase gradient of $k_g = \pi/8a$. (c) Mode profile on resonance when excited at normal incidence. The ellipses denote the geometry of the structure. (d) Far field for RCP incidence at each wavelength, demonstrating near-unity diffraction efficiency (96.1%) to the anomalously reflected angle (20.17°). The spin is preserved in transmission and reflection. (e) Far field for LCP incidence at each wavelength, showing no resonance.