Bound states in the continuum (BICs) are discrete eigenstates of open wave systems that are embedded in free-space radiation but completely orthogonal to the radiative continuum [1,2]. BICs are regarded as a universal wave phenomenon and have been extensively investigated in many research fields including electronics [3], acoustics [4], microwaves [5], and nanophotonics [6]. Recent advances in photonics reveal that some guided resonances could completely decouple from the radiative continuum, as a result of symmetry mismatch [7–9]. These radiative singularities were further identified as polarization vortices with integral topological charge [10]. One case of BICs is pinned at $\Gamma$ point as long as the structure symmetry is invariant, known as “symmetry-protected BICs” [11–14]. Another type of BICs could relocate, merge, or annihilate in $k$ space when tuning system parameters. These BICs are regarded as “accidental BICs” since they originate from accidental destructive interferences between different resonances [15,16]. Recently, the concept of BICs has boosted numerous applications in linear and nonlinear nanophotonics that leverage high-$Q$ resonances and strong electromagnetic (EM) energy confinements at the nanoscale. For example, Liu et al. proposed that ellipticity modulation of linear polarization could be achieved based on pairs of circularly polarized states spawn from BICs [17]. Huang et al. demonstrated an ultrafast BICs laser with the switching time reaching picoseconds level [18]. Wang et al. proposed guided resonances near BICs as orientation-variant wave plates in the momentum space and achieved a direct optical vortex generator that does not require central alignment [19].

Symmetry breaking is a vital and intriguing phenomenon that is related to nontrivial effects in many physical processes [20]. For example, breaking lattice inversion symmetry can transform Dirac points to Weyl points [21] and non-reciprocal wave propagation can be achieved by breaking time-reversal symmetry [22]. BICs could be transformed into quasi-BICs and achieve ultra-high-$Q$ resonances by tiny symmetry breaking of structures [11–14,23,24]. BICs result from the strong coupling between the resonant eigenstates in parameter space and appear as sharp Fano peaks (quasi-BICs) when they weakly couple to the radiative continuum [5,6,25–27]. By group theory analysis of eigenstate modes in momentum space, a road map was depicted for engineering far-field polarization of quasi-BICs [28]. Conventionally, nanostructures-based quasi-BICs mainly originate from in-plane or out-of-plane symmetry breaking of the building blocks. However, since the radiative $Q$ factor of quasi-BICs is proportional to the power inversion of asymmetry parameters [14], $Q$ factor is limited by certain geometric defects, leading to experimental challenges to realize the designed high $Q$ factors [24]. On the other hand, the space group of these devices degenerates into its subgroup when introducing defects into meta-atoms. These defects simultaneously break the symmetry elements and the space group of structures.

I. INTRODUCTION

Bound states in the continuum (BICs) are discrete eigenstates of open wave systems that are embedded in free-space radiation but completely orthogonal to the radiative continuum [1,2]. BICs are regarded as a universal wave phenomenon and have been extensively investigated in many research fields including electronics [3], acoustics [4], microwaves [5], and nanophotonics [6]. Recent advances in photonics reveal that some guided resonances could completely decouple from the radiative continuum, as a result of symmetry mismatch [7–9]. These radiative singularities were further identified as polarization vortices with integral topological charge [10]. One case of BICs is pinned at $\Gamma$ point as long as the structure symmetry is invariant, known as “symmetry-protected BICs” [11–14]. Another type of BICs could relocate, merge, or annihilate in $k$ space when tuning system parameters. These BICs are regarded as “accidental BICs” since they originate from accidental destructive interferences between different resonances [15,16]. Recently, the concept of BICs has boosted numerous applications in linear and nonlinear nanophotonics that leverage high-$Q$ resonances and strong electromagnetic (EM) energy confinements at the nanoscale. For example, Liu et al. proposed that ellipticity modulation of linear polarization could be achieved based on pairs of circularly polarized

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However, the exact relationship among the symmetry elements, space group, and the transition of quasi-BICs still needs to be investigated.

Metasurfaces are arrays of artificial subwavelength nanostructures that can sufficiently manipulate the EM fields at nanoscale [29]. With abundant local resonances enabled by the artificial nanostructures, such as Bragg resonances [30], Mie resonances [31,32], and surface plasmon polaritons [33], metasurfaces provide a versatile platform to realize holography, optical information multiplexing and possessing, and harmonic waves manipulation [34–38]. By combining the high Q nature of BICs and the EM fields manipulation of artificial nanostructures, the light-matter interaction efficiency of metasurfaces can be further enhanced, which can potentially lead to efficient applications in nonlinear and quantum physics. The ultra-high-Q resonances can be applied in various promising applications such as optical sensing and detecting since devices inspired by BICs have extremely high sensitivity and can achieve a lower detection threshold [39–41]. However, the current optical sensing methods are still limited to isotropic media, and to our knowledge, the anisotropic refractive index detection on the metasurfaces platform has not been explored yet. On the other hand, traditional resonance-shift-based sensing is not only affected by the refractive index of the media to be measured but also affected by environmental parameters such as temperature, cladding thickness, and surface roughness, which are challenging to be separated.

Here, we propose a multiband quasi-BICs transition method, which can realize the transition from ideal symmetry-protected BICs to quasi-BICs by breaking the symmetry elements of nanostructures and simultaneously identify the anisotropic refractive index and the thickness of a nanoscale layer. Different from previous works that require simultaneous symmetry breaking of meta-atoms and the space group to trigger the transition of quasi-BICs, we find that the out-coupling of BICs can be achieved by engineering the period of the metasurface, which changes specific symmetry elements (C2 and σ) of the nanostructure while keeping the space group invariant (pmm). Such perturbation enlarges the unit cell and enriches the eigenstates of ideal BICs, achieving multiband quasi-BICs. It is noted that researchers have achieved other nontrivial effects as well by enlarging the unit cell size of artificial microstructures, such as band inversion and topological edge states [42]. By tuning the asymmetry parameters in the x or y direction, a frequency-selective excitation of multiband quasi-BICs is achieved by different symmetries of eigenstate fields. Furthermore, the identification among birefringent refractive indices and cladding thickness can be realized based on the proposed quasi-BICs transition method.

II. DESIGN OF QUASI-BICS

The schematic of the proposed metasurface composed of silicon nanoboxes and a SiO2 substrate is shown in Figs. 1(a) and 1(b). We consider four identical nanoboxes as the unit cell of our periodic planar structure. The gaps sizes g inside the unit cell in both x and y directions have the same value and remain invariant, which are fixed at g = 120 nm. The periods in x and y directions of the original metasurface are set as px = 800 nm and py = 660 nm. When the gap size meets the condition g1 = g2 = g, a single nanobox can also be considered as a unit cell. The refractive index of SiO2 is set as 1.5 and the permittivity of Si in the near-infrared wavelengths is adopted from experimental data of Palik [43]. Conventionally, the transition from symmetry-protected BICs to quasi-BICs is triggered by introducing defects into metasurfaces that simultaneously breaks the symmetry elements and the space group of structures [11–14]. In our design, we can alternatively trigger the transition from BICs to quasi-BICs by perturbing the periods (px or py) at around 800 nm and 660 nm, respectively, or the gap sizes (g1 or g2) at around 120 nm) for the perturbed metasurface. This kind of symmetry breaking does change symmetry elements of nanostructures
such as half turns ($C_2$) pinned at the center of the nanobox (indicated by white dots) and mirror axes ($\sigma_x$ and $\sigma_y$) connecting these $C_2$ points (dashed lines), while keeping the entire space group isomorphism invariant ($pmm$) [44]. The band diagram of the original metasurface is shown in Fig. 1(c). We focus on the lowest band shown as the blue line. To clearly show the origination of this band, the multipole contributions of the eigenstate field are analyzed [45]. We expand the scattering energy to the first four items, namely electric dipole (ED), magnetic dipole (MD), electric quadrupole (EQ), and magnetic quadrupole (MQ). The results show that nearly 99% of the scattering energy comes from MD. Combining the eigenstate field distribution in the inset of Fig. 1(c), we confirm that the MD oscillates along the $z$ direction, which cannot be excited by a normally incident plane wave. Since the nondegenerate bound state at the $\Gamma$ point resides in the radiation continuum, it is considered a BIC [46]. By merely breaking the aforementioned symmetry elements of the nanostructures, the radiation leakage of ideal BICs modes towards free space can be achieved, appearing as sharp Fano peaks as shown in Fig. 1(f) (one of the quasi-BICs resonances shown for simplicity).

As a result of perturbation on the periods, the eigenstates and ideal BICs are enriched. The eigenstate field at $\Gamma$ point of the perturbed metasurface in Figs. 1(e) and 1(f) could be understood as bonding and antibonding hybridization of the characteristic resonant modes of the constituent nanoboxes, which is analogous to the plasmon hybridization [47]. The symmetries of resonant eigenstates correspond to irreducible representations of the $C_{2v}$ point group, namely two anti-symmetric $B$ representations (for modes i and ii) and two symmetric $A$ representation (for modes iii and iv), as shown in Fig. 1(f). Thus, ideal BICs modes can be theoretically enriched by four times for different hybridization of eigenstate field, achieving multiband quasi-BICs. The eigenstate field distributions shown in Fig. 1(f) also distinguish out-of-plane $C_2$ symmetries ($C'_2$ or $C''_2$), and they are BICs protected by different symmetries. The bands and the eigenstate field distributions in this paper are obtained by finite-element-method (FEM) eigenvalue solver in COMSOL Multiphysics. The solver searches the eigenvalues around 300 THz. The relative computing errors of solutions are lower than $10^{-6}$. We did not consider the effects of substrate in Fig. 1 to obtain the ideal dipole decomposition in theory. To show the ideal BICs, we set the same parameter values for the original and perturbed metasurfaces ($g_1 = 820$ nm, $g_2 = 680$ nm, solid lines) and the perturbed metasurface ($g_1 = 820$ nm and $g_2 = 680$ nm, dashed lines) by normal incident plane waves. $E_i$ implies the incident polarization ($i = x, y$). (b),(c) EM fields distributions at different resonant modes ($M_{A1}, M_{A2}$) with $x$-polarized incident light. (d)–(f) EM fields distributions at different resonant modes ($M_{B1}, M_{B2}$, and $M_{B3}$) with $y$-polarized incident light. The EM fields are depicted in the $x$-$y$ cutplane bisecting the nanoboxes and are normalized to the incident EM fields intensity. The color maps depict magnetic (electric) field enhancement for mode $M_{A1}$, and $M_{B3}$ ($M_{A2}$, $M_{B1}$, and $M_{B2}$), and white arrows depict electric (magnetic) field.

III. RESULTS AND DISCUSSIONS

The perturbations of the periods ($p_x = 820$ nm, $p_y = 680$ nm) enable BICs to appear as ultrasharp Fano line-shapes, achieving multiband quasi-BICs excitation as shown in Fig. 2(a). The Fano line-shapes disappear when the disorders are removed. The quasi-BICs resonances of $M_{Ai}$ ($i = 1, 2$) and $M_{Bj}$ ($j = 1, 2, 3$) correspond to $x$- and $y$-polarized incident light, respectively. For the transverse electric (TE) mode in Fig. 2(b), mode $M_{A1}$ consists of four MD modes oriented along the $z$ direction, with in-phase (out-of-phase)
hybridizations in the $x$ ($y$) direction. Similarly, mode $M_{B3}$ plotted in Fig. 2(f) can be understood as hybridization of MD modes in the opposite way. The transverse magnetic (TM) modes $MA_2$ and $MB_2$ can be decomposed into in-phase and out-of-phase EDs as well [see Figs. 2(c) and 2(e)]. Different from the four modes discussed above, mode $M_{B1}$ consists of four MDs along the $y$ direction, oriented antiparallelly in both the $x$ and $y$ directions, as shown in Fig. 2(d). Besides, the electric field of resonance mode $M_{B1}$ is mostly localized around the structure gap, and the normalized electric field amplitude $|E/E_0|$ is enhanced by more than $10^2$ times, which is desirable for applications such as optical sensing and harmonic generation.

Along with symmetry breaking, BICs transform to quasi-BICs, leaking lights to free space and with $Q$ factors decreasing drastically [14]. This is a typical characteristic of quasi-BICs and is important for realistic applications. The Fano lineshape evolutions as a function of asymmetry parameters $p_x$, $p_y$, or $\delta p$ are demonstrated in Figs. 3(a)–3(e), where $\delta p$ denotes the same perturbation of $p_x$, and $p_y$, deviated from 800 nm and 660 nm, respectively. The reflection spectra show that the linewidths of these five peaks expand wider for larger asymmetry parameters. The narrow lineshapes will disappear if the symmetry disorder is zero, indicating ideal BICs. Additionally, the linear-polarized plane waves can selectively stimulate quasi-BICs modes $MA_1$ and $MB_2$ by only tuning $p_y$ [see dashed lines in Fig. 3(f)]. In the case of perturbing both $p_x$ and $p_y$, all five quasi-BICs modes could be excited by linear-polarized incident light, as aforementioned in Fig. 2(a). Thus, selective excitation of multiband quasi-BICs can be achieved by tuning one or two asymmetry parameters.

To explain the selective excitation effects, we further investigate the free-space-coupling behaviors of BICs when tuning asymmetry parameters as shown in Fig. 4. We take mode $MA_1$, $MA_2$, and $MB_1$ as examples. One of the intuitive physical quantities to estimate free-space out-coupling is the radiative $Q$ factor of resonances. As shown in Figs. 4(a)–4(c), we simulated the two-dimensional (2D) maps of the $Q$ factor as a function of both $p_x$ and $p_y$ [$Q(p_x, p_y)$]. The $Q$ factors are derived from calculated complex eigenfrequencies of the modes using FEM. We can see their different behaviors, which are consistent with the selective excitation in spectra in Fig. 3. For the BICs mode $MA_1$ shown in Fig. 4(a), $p_x$ barely affects its $Q$ factor while the $Q$ factor drastically decreases when $p_y$ deviates from 660 nm (the parameter value of the original metasurface). For the mode $MA_2$, the effects of $p_x$ and $p_y$ will exchange. For the mode $MB_1$, we could only trigger the transition from BICs to quasi-BICs by simultaneously modulating $p_x$ and $p_y$. The ultra-high-$Q$ pale yellow regions in Figs. 4(a)–4(c) depict different BICs shapes, indicating that symmetry breaking requires different asymmetry parameters in these ideal BICs modes.

The out-of-phase hybridization of modes brings in distinct symmetries. In Figs. 4(d)–4(f) we illustrate the eigenstate fields of BICs corresponding to modes $MA_1$, $MA_2$, and $MB_1$. For mode $MA_1$, as long as the out-of-phase condition is satisfied, the MD radiations will be perfectly canceled in the far field through destructive interferences, forming symmetry-protected BICs. It is noted that the out-of-phase hybridization introduces out-of-plane $C_2$ axes along the $x$ direction ($C_2^x$) in the $x$-$y$ eigenstate fields cutplane. Thus, merely perturbing $p_x$ does not break the symmetry elements and could not trigger the transition of quasi-BICs. Similarly, BICs mode $MA_2$ possesses out-of-plane $C_2$ axes along the $y$ direction ($C_2^y$). The effects of $p_y$ and $p_x$ exchange for mode $MA_2$. BICs mode $MB_1$ owns out-of-plane $C_2$ axes in both $x$ and $y$ directions ($C_2^x$ and $C_2^y$). We can transform BICs mode $MB_1$ to quasi-BICs by simultaneously breaking symmetry elements $C_2^x$ and $C_2^y$. Such relationship between symmetry and quasi-BICs transition demonstrates that the selective excitation of quasi-BICs is

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FIG. 3. Fano lineshapes evolution versus asymmetry parameters and selective excitation of multiband quasi-BICs. (a),(b) Reflection spectra of designed metasurface as a function of $p_y$ with $y$- and $x$-polarized incidence, where $p_y = 800$ nm. The black arrows are an eye guide to show the degree of symmetry breaking and the gray regions represent the original metasurface. (c),(d) Reflection spectra of the perturbed metasurface as a function of $p_y$ with $y$- and $x$-polarized incidence, where $p_y = 660$ nm. (e) Reflection spectra of the perturbed metasurface as a function of $\delta p$ with $y$-polarized incident plane waves. Note that this case is the same as Fig. 2(a), which means all five quasi-BICs modes could appear if both $p_x$ and $p_y$ are perturbed. (f) Reflection spectra in the case of $p_x$ and $p_y$ with larger wavelength range, to show clearly that only one quasi-BIC can be excited in the operating spectral region by $x$- or $y$-polarized plane waves.
FIG. 4. Eigenmode calculation and coupling strength analysis by in-plane ED moment. (a)–(c) $Q$ factor maps of BICs mode $M_{A1}$, $M_{A2}$, and $M_{B1}$ supported by designed metasurface as a function of $p_x$ and $p_y$. (d)–(f) EM fields distributions of eigenmode $M_{A1}$, $M_{A2}$, and $M_{A1}$ supported by the original metasurface. Out-of-plane components of EM fields are plotted as color maps and the corresponding in-plane components are depicted by arrows (white arrows for TE modes and black for TM modes). Light blue lines represent out-of-plane half turns $C_2^x$ and $C_2^y$. (g)–(i) In-plane ED moment components $P_x$ (solid lines) and $P_y$ (dashed lines) versus asymmetry parameters $p_x$ (blue lines), $p_y$ (red lines), and $\delta p$ (black lines).

determined by the symmetry of eigenstate fields (irreducible representations).

To more quantitatively estimate eigenstate free-space out-coupling, one can employ the overlapping between incident wave field and eigenstate field. We assume $e^{-i\omega t}$ time dependence of EM fields and express the eigenstate field in the form of current density. The coupling strength $c$ can be written as [48]:

$$c \propto \int_V [j(r) \cdot E] e^{ikz} \, d\mathbf{r}, \quad (1)$$

where $V$ is the volume of silicon boxes, $j(r)$ is the current density of eigenstate field, and $E e^{ikz}$ represents a normal incidence plane wave with a wave vector $k$ along the $z$ direction and with polarization vector $E$ in the $x$-$y$ plane (a unit vector). The integral in Eq. (1) generates the total ED moment of the entire structure. For unperturbed nanostructures such as the original metasurface,

$$c \propto P \cdot E = 0 \quad (2)$$

is the condition for ideal symmetry-protected BICs. The symmetry disorders can result in the eigenstate field in the nanostructures coupling to radiative plane waves for $x$ or $y$ polarization. The $x$ and $y$ components of coupling strength can be expressed as:

$$c_{x,y} \propto P \cdot E_{x,y} = P_{x,y}. \quad (3)$$

Thus, the zero-order-diffraction quasi-BICs in periodic nanostructures cannot be excited unless the eigenstate near-field generates in-plane ED moment.

The variations of in-plane components of ED moment $P_x$ and $P_y$ as a function of asymmetry parameters $p_x$, $p_y$, or $\delta p$ are depicted in Figs. 4(g)–4(i). For BICs mode $M_{A1}$, ED moment remains zero when only tuning $p_x$. The ED moment increases from zero as $p_y$ deviates from 660 nm (the parameter value of the original metasurface), as shown in Fig. 4(g). For mode $M_{A2}$, the effects of $p_x$ and $p_y$ will exchange, as plotted in Fig. 4(h). For BICs mode $M_{B1}$ [see Fig. 4(i)], a total in-plane ED moment (along the $y$ direction) will not appear unless simultaneously perturbing both asymmetry parameters $p_x$ and $p_y$. The in-plane EM multipole analyses are in good agreement with $Q$ factor evolution in Figs. 4(a)–4(c) and reflection spectra in Fig. 3. It is worth noting that the overlapping between eigenstate field and the incident light can be applied in structured light (e.g., vector beams) as well, when the coupling strength is attributed to high-order EM multipoles.

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TABLE I. Symmetry of multiband BICs and broken symmetry elements in quasi-BICs.

<table>
<thead>
<tr>
<th>BICs modes</th>
<th>Space group</th>
<th>Point group</th>
<th>Irreducible representations</th>
<th>Broken symmetry elements in quasi-BICs</th>
</tr>
</thead>
<tbody>
<tr>
<td>M_A1</td>
<td>pmm</td>
<td>C_2v</td>
<td>B_1</td>
<td>C'_2</td>
</tr>
<tr>
<td>M_A2</td>
<td>pmm</td>
<td>C_2v</td>
<td>B_2</td>
<td>C'_2</td>
</tr>
<tr>
<td>M_B1</td>
<td>pmm</td>
<td>C_2v</td>
<td>A_2</td>
<td>C'_2, C'_2</td>
</tr>
<tr>
<td>M_B2</td>
<td>pmm</td>
<td>C_2v</td>
<td>B_1</td>
<td>C'_2</td>
</tr>
<tr>
<td>M_B3</td>
<td>pmm</td>
<td>C_2v</td>
<td>B_2</td>
<td>C'_2</td>
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</table>

We also summarize the symmetry of multiband BICs and the broken symmetry elements in quasi-BICs in Table I. The point group and space group of the original metasurface and the perturbed metasurface remain invariant. Due to the intrinsic symmetry distinction (irreducible representations) of ideal BICs, quasi-BICs in the perturbed metasurface are triggered by breaking different symmetry elements ($C'_2$ or/and $C'_2$).

We also propose a sensing method based on the multiband resonances with high-$Q$ factors to distinguish among birefringence refractive indices $n_{o}$, $n_{e}$, and cladding thickness. The diagram of the proof-of-concept is illustrated in Fig. 5(a). The nanoboxes metasurfaces are covered by an anisotropic medium, which is higher than the nanoboxes by $\delta h$. For simplicity, we take uniaxial crystals as an example. Generally, spectral locations and $Q$ factors of resonances are functions of the cladding refractive indices and the thickness, i.e., $\lambda_1(n_{o}, n_{e}, \delta h)$, $Q_1(n_{o}, n_{e}, \delta h)$, $\lambda_2(n_{o}, n_{e}, \delta h)$, $Q_2(n_{o}, n_{e}, \delta h)$, etc. Each of the functions is a different sensing channel and supports a different degree of freedom in a sensing problem. The more sensing channels, the more precise sensing would be. To avoid a complicated three-dimensional fitting, we first use dual resonances location channels to sense $n_{e}$ and $n_{o}$, utilizing quasi-BICs mode $M_{A1}$ and $M_{B1}$. From the 2D fitting plots shown in Figs. 5(b) and 5(c), we can see a well-fitted blue plane to the calculated red dots representing resonance peaks. In Figs. 5(d) and 5(e), we show $Q$ factor linear fitting of refractive indices ($n_{o}$, for example) at different cladding thicknesses. The $Q$ factors of BICs modes $M_{A1}$ and $M_{B2}$ are derived through Fano lineshape fitting and are hardly dependent on refractive indices. In contrast, the $Q$ factors vary significantly when modulating the cladding thickness. These results indicate that we could separate cladding thickness ($\delta h$) and refractive indices ($n_{o}$, $n_{e}$) by measuring resonance $Q$ factors. Thus, we can employ the spectral locations and $Q$ factors of multiband quasi-BICs to sense birefringence refractive indices $n_{o}$, $n_{e}$ and the cladding thickness $\delta h$, achieving multivariable optical sensing.

IV. CONCLUSION

In conclusion, we propose an approach that can transform symmetry-protected BICs to quasi-BICs by merely breaking specific symmetry elements of nanostructures, namely in-plane half-turns $C_2$ and mirror axes $\sigma$. Instead of breaking symmetry elements and space groups simultaneously, our approach modulate the periods of metasurfaces and introduce a disorder in the size of the unit cell while keeping the space group invariant. Precisely controlling periods of fabricated nanostructures is generally considered to be more convenient and more accurate than tiny defects in meta-atoms, and the $Q$ factor of flat devices is expected to be further improved. Apart from triggering the transition from ideal BICs to quasi-BICs, the perturbation of the periods enlarges the unit cell as well, which enriches the ideal BICs, achieving multiband quasi-BICs. Besides, selective excitation of multiband quasi-BICs is achieved by tuning the asymmetry parameters and is explained by the irreducible representation of eigenstate field. Some works were devoted to generate accidental BICs or Friedrich-Wintgen BICs by nonperiodic structures [2,5,25] and parameter tuning [49]. We elucidated the relationships among symmetry elements, space group symmetry, and the transition from symmetry-protected BICs to quasi-BICs.
which are rarely discussed in the previous works. Based on the multiband high-\(Q\) resonances, a precise sensing mechanism is proposed to detect claddling birefringence refractive indices and thickness, achieving multivariable optical sensing that may be applicable for engineering dynamic metasurfaces (e.g., infiltrated by liquid crystals [50]). The proposed scheme can be further expanded to nonlinear and quantum photonics, and benefits applications from giant harmonic generations, low-threshold lasers, biosensing to photonic circuits.

ACKNOWLEDGMENTS

This work was supported by the National Key Research and Development Program of China (2016YFA0301102 and 2017YFA0303800), the National Natural Science Foundation of China for Distinguished Young Scholars (1925403), the National Natural Science Foundation of China (11904183, 11904181, 11974193, 91856101, and 11774186), and the Natural Science Foundation of Tianjin for Distinguished Young Scientists (18JCQJC45700).


