

Tailoring bound states in the continuum in photonic crystal slabs via lattice engineering

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Bound states in the continuum (BICs) enable strong light confinement and enhanced light-matter interactions, yet how lattice deformation governs their momentum-space evolution remains unclear. Here, we develop a lattice-engineering framework for silicon photonic crystal slabs by investigating the continuous evolution from a square lattice to rectangular and monoclinic lattices. A symmetry-constrained far-field expansion shows that rectangular deformation lifts the degeneracy between two orthogonal BIC branches, while the preserved mirror symmetries pin their trajectories to the principal axes. Near the merging point, k_{BIC}^2 varies linearly with the aspect-ratio detuning. Monoclinic shear removes these mirror constraints and enables coupling between orthogonal momentum components, steering the BICs along off-axis trajectories. The slab thickness provides an additional degree of freedom to shift the BICs along these symmetry-allowed trajectories and drive their charge-conserving merging at the Γ point. Further breaking the in-plane C_2 symmetry of the unit cell splits integer-charge BICs into circular-polarization points carrying half-integer topological charges, accompanied by extended regions of high ellipticity. These results show how lattice symmetry constrains BIC trajectories and geometric tuning controls their positions, providing a route to engineering BIC merging and polarization singularities.

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I. INTRODUCTION

Bound states in the continuum (BICs) have emerged as a revolutionary concept in photonics, providing unique opportunities for manipulating light at the nanoscale [1–4]. Originally introduced in quantum mechanics [5], BICs have been extended to electromagnetic waves [6–9], acoustics [10–12], and elastic waves [13], highlighting their versatility across various wave phenomena. BICs are characterized as trapped modes with infinite quality (Q) factors, even though they reside within the radiation continuum, making them ideal for confining light without any radiation loss. Their remarkable ability to trap light and decoupling from far-field radiation allows for the complete isolation of these modes from external excitations, which is crucial for applications requiring extreme light confinement. In practical systems, BICs should be converted into quasi-BICs (QBICs) by introducing perturbations, where the modes exhibit finite but extremely high Q-factors [14]. The excitation of QBICs often results in substantial field enhancements, rendering them highly desirable for a wide range of photonic and optoelectronic devices [15], such as lasers [16–18], biosensors [19–22], modulators [23], thermal emitters with high coherence [24–27], and high-harmonic generation [28–31].

BICs are also fundamentally linked to polarization singularities in the momentum space [32], where each BIC carries an integer topological charge. This association provides additional freedom for tailoring the properties of electromagnetic waves, such as amplitude and polarization, enabling novel functionalities like vortex beam generation [33,34] and chiral optics [35–40]. Furthermore, merging multiple BICs into a super-BIC can significantly improve the robustness of Q-factors against variations in incident angles and topological disorder [41–43]. The combination of these properties makes BICs a powerful platform for boosting light-matter interaction [44,45].

To date, the majority of studies on BICs have focused on periodic structures with either a C_{4v} or C_{6v} symmetry, such as photonic crystal slabs (PCSs) [6,42,43,46,47] and metasurfaces [48–51] with either square [6,46,50] or hexagonal lattices [52,53]. Beyond these high-symmetry configurations, BICs can be manipulated by modifying the shape or orientation of the constituent meta-atoms and thereby reducing the unit-cell symmetry [54,55]. Such symmetry-breaking approaches can split integer-charge BICs into half-charge C-points, control the generation and annihilation of circularly polarized states, and enable unidirectional guided resonances or intrinsic chiral BICs [53,56–58]. At the lattice level, monoclinic arrangements have also been employed to construct chiral QBICs and generate pronounced chiral dichroism [39,59].

Recent studies have further revealed richer topological-charge dynamics, including half-integer polarization

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singularities associated with quasi-Dirac BICs [60], radiation-channel-dependent topological charges in Janus BICs [61], perturbation-induced displacement of BIC polarization vortices [62], and robust chirality obtained by merging accidental BICs with a net zero topological charge [40]. These results demonstrate that the motion, splitting, and merging of BICs can originate from distinct symmetry, band-topology, and radiation-channel mechanisms. Nevertheless, the role of continuous Bravais-lattice deformation in reorganizing the trajectories and merging of multiple BICs remains insufficiently understood. In particular, a unified description connecting square, rectangular, and monoclinic lattices to the corresponding symmetry constraints on BIC motion is still lacking.

In this work, we systematically explore the evolution of BICs in PCSs through continuous lattice transformations from square to rectangular and monoclinic lattices. We show that the BICs along the x -axis are compressed toward the Γ point and merge into a single super BIC as the square lattice is gradually transformed into a rectangular lattice by adjusting the aspect ratio. A symmetry-based semianalytical model further reveals that, near the merging condition, the squared BIC position varies linearly with the aspect-ratio detuning, providing a direct relation between the lattice geometry and the BIC position. We further demonstrate that in a PCS with a monoclinic lattice two BICs with a topological charge of $q = -1$ at off- Γ points merge with a BIC with $q = +1$ to form a new BIC with $q = -1$ when the included angle decreases from 90° to 85° . Further reducing the thickness allows these merged BICs to converge at the Γ point. In addition, we show that multiple circularly polarized states (C-points) can be generated and manipulated by breaking C_{2v} symmetry of the monoclinic lattice by replacing the circular hole with a crescent-shaped hole. By choosing the proper thickness, an extended high-ellipticity region can be formed over a broad range of wave vectors. Besides, we explore the effect of the rotation of crescent-shaped air holes on BICs. Simulation results indicate that these BICs undergo dynamic splitting and merging multiple times as they rotate around the Γ point. Finally, we show that BICs can also be manipulated by a PCS with a rotated elliptical hole in the unit cell. Our work establishes a symmetry-guided framework for controlling the positions, trajectories, and merging of BICs through continuous lattice engineering, with further extensions to the manipulation of polarization singularities.

II. NUMERICAL METHODS

All numerical calculations were performed using the finite-element eigenfrequency solver in COMSOL MULTIPHYSICS with the Electromagnetic Waves, Frequency Domain interface. A single primitive unit cell was employed, with Bloch-Floquet periodic boundary conditions imposed on the in-plane boundaries. The computational domain normal to the photonic crystal slab was terminated by perfectly matched layers to describe outgoing radiation.

Because the structures considered here preserve mirror symmetry with respect to the middle plane of the slab, only one half of the structure was modeled. A perfect magnetic conductor (PMC) boundary condition was imposed at the

middle plane to select the TE-like modes, whereas a perfect electric conductor (PEC) boundary condition was used for the TM-like modes. The silicon slab and the surrounding medium were described by refractive indices of $n_{\text{Si}} = 3.48$ and $n_{\text{bg}} = 1.46$, respectively. Both materials were assumed to be lossless and dispersionless within the frequency range considered. The radiative quality factor was obtained from the complex eigenfrequency,

$$Q_{\text{rad}} = \frac{\text{Re}(\omega)}{2|\text{Im}(\omega)|}. \quad (1)$$

Since material absorption was neglected, the calculated quality factor corresponds to the radiative quality factor. The complex amplitudes of the zeroth-order radiation channels, c_x and c_y , were extracted from the spatial Fourier components of the electromagnetic field on a horizontal surface located in the homogeneous background region between the slab and the PML. The Stokes parameters were calculated as

$$S_0 = |c_x|^2 + |c_y|^2, \quad S_1 = |c_x|^2 - |c_y|^2, \quad (2a)$$

$$S_2 = 2\text{Re}(c_x c_y^*), \quad S_3 = -2\text{Im}(c_x c_y^*). \quad (2b)$$

The normalized ellipticity was defined as $\rho = S_3/S_0$. Here, $\rho = 0$ signifies pure linear polarization, while $\rho = \pm 1$ corresponds to right-handed (RCP) and left-handed (LCP) circular polarization states, respectively.

Ideal BICs were first identified from momentum-space Q -factor maps and were subsequently refined through local wave-vector and structural-parameter scans. Representative mesh-convergence tests and the coarse-to-fine procedure used to determine the BIC merging condition are provided in Figs. S6 and S4, respectively, in Supplemental Material (SM) [63].

III. RESULTS AND DISCUSSION

We consider a silicon PCS with a square lattice, as schematically shown in Fig. 1(a). The structural parameters of the PCS are set as follows: lattice constant $a = 519.25$ nm, thickness $t = 600$ nm, and air hole diameter $D = 175$ nm. Unless otherwise specified, the material properties and numerical settings are those described in the Numerical Methods section. Figure 1(b) shows the band structure of this PCS. Here, we focus on the lowest-order mode, namely the TE_1 mode marked by the red line in the figure. Figure 1(c) shows the magnetic field distribution of this mode. Previous studies have demonstrated that such a PCS hosts nine BICs in the momentum space [34], including eight accidental BICs distributed at the $k_x(k_y)$ axis and diagonal (antidiagonal) and one symmetry-protected (SP) BIC at Γ point. By either reducing the thickness to $t = 582$ nm or adjusting the lattice constants to $a = 534.5$ nm, these BICs can be merged into a super BIC, whose Q -factor follows a scaling law $Q \propto k^{-6}$ in the vicinity of Γ point, as depicted in Fig. 1(g). Here, the red color represents the Q -factor along the k_x axis and the blue color denotes the Q -factor along the k_y axis. Owing to the lattice symmetry, the Q -factor distributions along the k_x and k_y axes are identical.

Subsequently, the lattice type is intentionally transformed from a square lattice to a rectangular configuration by tuning the ratio between two lattice constants (defined as the aspect

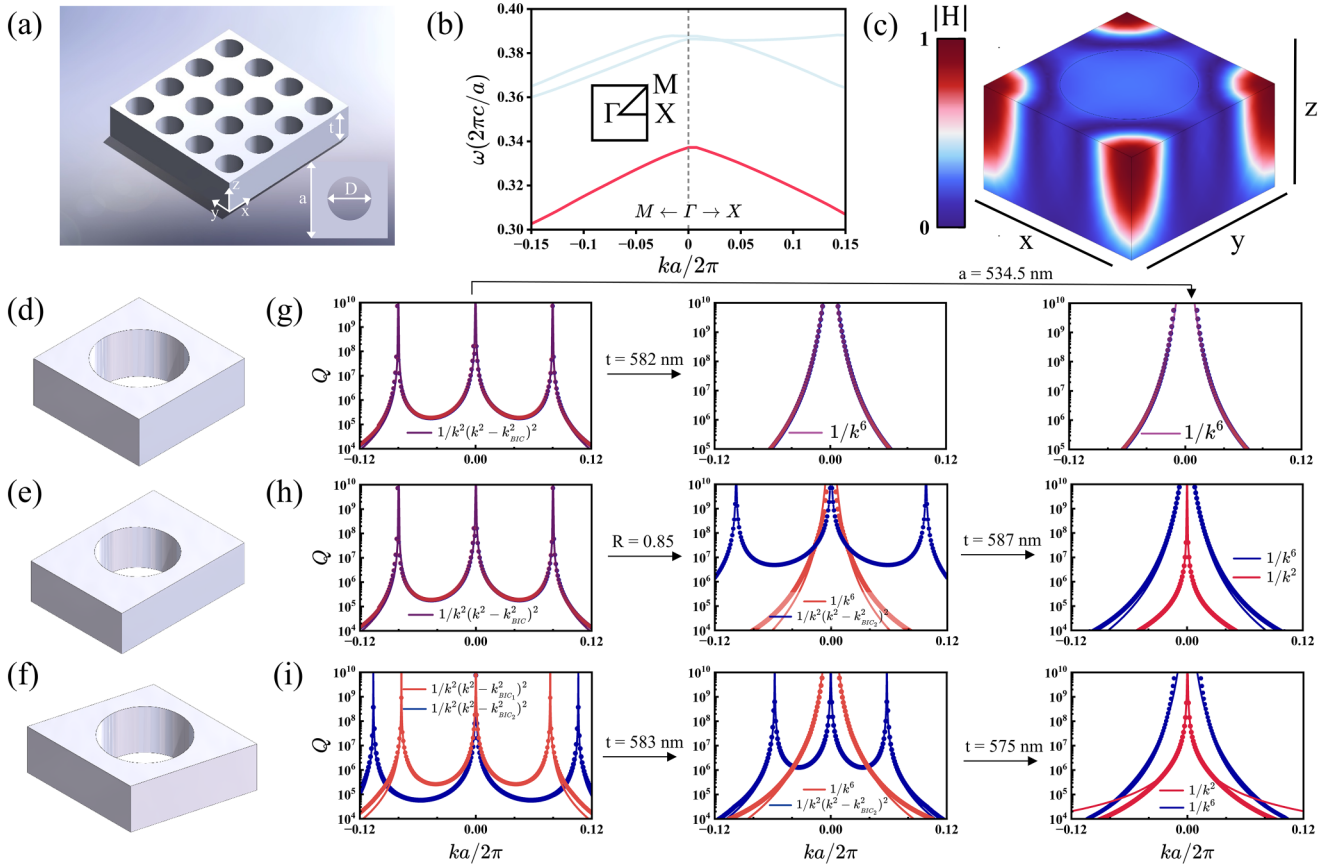


FIG. 1. BIC evolution in a PCS with various lattice types. (a) Schematic of the PCS. (b) Band structure of a PCS with a square lattice. (c) Magnetic field distribution of BIC at Γ point. [(d)–(f)] Structural schematic of the square (d), rectangular (e), and monoclinic (f) lattice PCS. [(g)–(i)] BIC merging behavior in the square (g), rectangular (h), and monoclinic (i) lattices.

ratio $R = b/a$ while keeping the unit cell area unchanged, as shown in Fig. 1(e). When the aspect ratio is adjusted to $R = 0.85$, the BICs along the k_x axis are found to merge at the Γ point, with the Q-factor following a scaling law $Q \propto k^{-6}$, whereas the positions of BICs along the k_y axis remain almost unchanged. A further reduction in the thickness to $t = 587$ nm results in the merging of BICs along the k_y axis at the Γ point, whose Q-factor also obeys a scaling law $Q \propto k^{-6}$. In contrast, the Q-factor distribution of BICs along the k_x axis is reduced to $Q \propto k^{-2}$ after merging, as shown in Fig. 1(h).

We also study BIC evolution as the lattice type is varied from a square lattice to a monoclinic lattice, while the area of the unit cell remains unchanged. We assume the four sides of the lattice to be of equal length and only tune the included angle θ between two sides. At $\theta = 85^\circ$, the BICs exhibit an anisotropic distribution along the diagonals in momentum space. Gradually tuning the thickness of PCS enables the construction of anisotropic BIC merging, as demonstrated in Fig. 1(i). In the following, we present more detailed discussions on BIC evolution as the lattice types vary.

Since each BIC is also a vortex center of far-field polarization in momentum space, the topological charge is introduced to characterize the topological nature of BICs. The topological charge q is defined as the winding number of the far-field radiation vector, $q = \frac{1}{2\pi} \oint \mathbf{k}_\parallel \cdot \nabla_{\mathbf{k}_\parallel} \phi(\mathbf{k}_\parallel)$, where the integration is performed along a closed loop in momentum space around the polarization-vortex center, $\mathbf{c}(\mathbf{k}_\parallel) = c_x(\mathbf{k}_\parallel)\mathbf{i} + c_y(\mathbf{k}_\parallel)\mathbf{j}$

is the polarization vector projected onto the xoy plane, $\phi(\mathbf{k}_\parallel) = \frac{1}{2} \arg[S_1(\mathbf{k}_\parallel) + iS_2(\mathbf{k}_\parallel)]$ and is the angle between the major axis of the far-field polarization ellipse and the x axis.

When the lattice type of a PCS is switched from a square lattice to a rectangular one, rich topological dynamics are found in Fig. 2. Figure 2(a) presents the magnetic field distribution (at $z = 0$) of BIC at Γ point in the PCS with a rectangular lattice. At $R = 1$ (square lattice), nine BICs can be observed in the momentum space from Fig. 2(c), including one SP-BIC with a topological charge $q = +1$ at the Γ point, four accidental BICs (A-BICs) with $q = -1$ at $\mathbf{k} = k_0[\cos(\frac{m\pi}{2})\hat{x} + \sin(\frac{m\pi}{2})\hat{y}]$, and another four A-BICs with $q = +1$ at $\mathbf{k} = k_0[\cos(\frac{(2m-1)\pi}{4})\hat{x} + \sin(\frac{(2m-1)\pi}{4})\hat{y}]$. (where k_0 is a constant and $m = 1, 2, 3$, and 4). Figures 2(c)–2(f) show that as R decreases from 1 to 0.85, the A-BICs on both sides move toward the central axis in a transversely compressed manner and eventually merge horizontally along the central axis. Specifically, two A-BICs with $q = +1$ merge with one A-BIC with $q = -1$ to form a single super BIC with $q = +1$ on both the upper and lower sides of the axis. Meanwhile, the SP-BIC with $q = +1$ at the Γ point merges with the A-BICs with $q = -1$ on the left and right sides to form a new SP-BIC with $q = -1$ at the Γ point.

Next, we further tune the thickness of the PCS with the aspect ratio fixed at $R = 0.85$. As the thickness decreases from 600 to 570 nm, the A-BICs with $q = +1$ on the upper and lower sides move toward the Γ point and ultimately merge

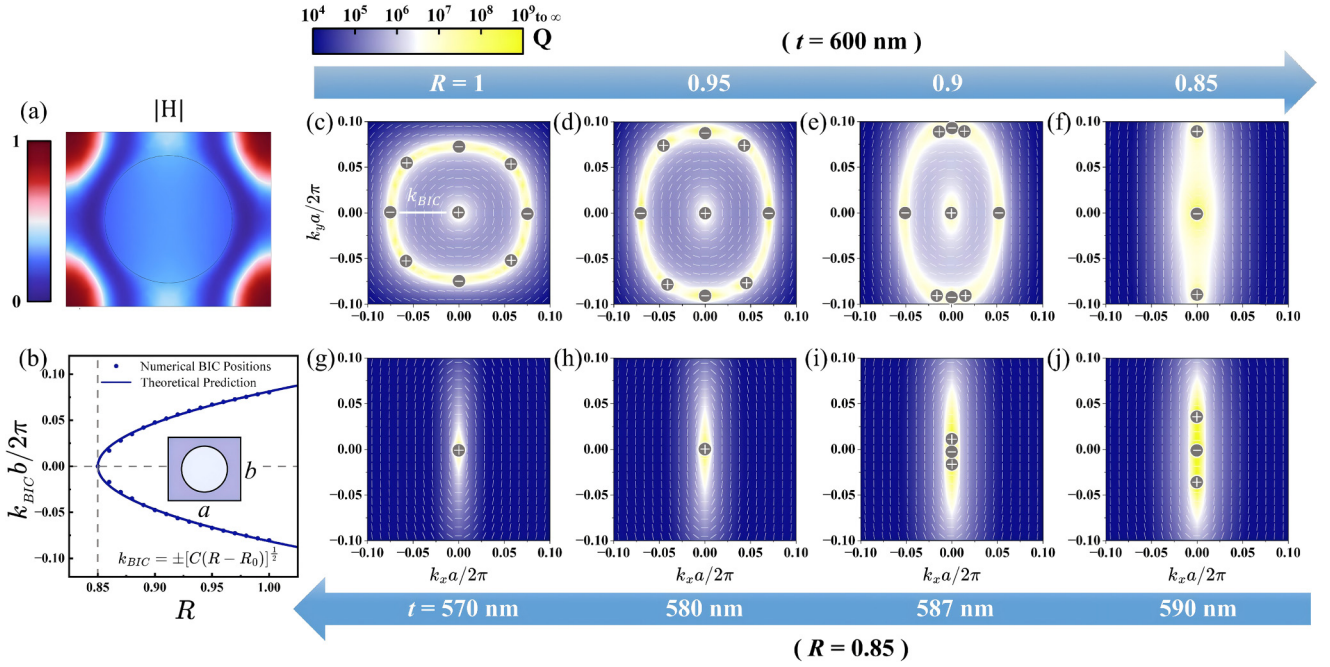


FIG. 2. BIC evolution in rectangular lattice PCS under lattice and thickness engineering. (a) Eigenfield distribution of the Hz component in the rectangular lattice. (b) Square-root dependence of the normalized BIC position $k_{BIC}b/2\pi$ on the aspect ratio detuning. [(c)–(f)] Evolution of BICs in momentum space showing transverse merging as the aspect ratio R decreases from $R = 1$ to 0.85. [(g)–(j)] Evolution of BICs in momentum space showing longitudinal merging when the thickness t is $t = 570$ (g), 580 (h), 587 (i), and 590 (j), while the aspect ratio is fixed as $R = 0.85$.

into a single SP-BIC with $q = +1$ at the Γ point. In addition, we calculate the critical wave vector k_{BIC} of forming A-BICs along k_x axis at different R . Surprisingly, we find that the squared BIC position varies linearly with the aspect-ratio detuning. This indicates that we can precisely engineer the longitudinal positions of A-BICs in momentum space by simply adjusting the lattice aspect ratio via lattice engineering, and then manipulate their transverse positions in momentum space by tuning the slab thickness. Through the synergistic modulation of the aspect ratio and thickness, we can realize customized BICs over a broad symmetry-allowed region of momentum space based on such a PCS.

To provide a physical interpretation of the observed evolution of A-BICs and the linear dependence of k_{BIC}^2 on the aspect ratio tuning, a symmetry-based semianalytical framework is developed based on the far-field radiation-zero condition. In the momentum space, a BIC is identified as a zero of the far-field radiation vector $\mathbf{c}(\mathbf{k}, R) = (c_x, c_y)$ [32,43,64]. For a rectangular lattice, the C_{2v} symmetry preserves the mirror symmetries with respect to the x and y axes, so that the far-field amplitudes near Γ point can be written as

$$c_x = k_x[\alpha_x(R) + \beta_x(R)k_x^2 + \gamma_x(R)k_y^2 + \dots], \quad (3a)$$

$$c_y = k_y[\alpha_y(R) + \beta_y(R)k_y^2 + \gamma_y(R)k_x^2 + \dots]. \quad (3b)$$

Along the high-symmetry line $k_y = 0$, the BIC condition reduces to $c_x = 0$, yielding the off- Γ branch

$$k_{BIC, x}^2 = -\frac{\alpha_x(R)}{\beta_x(R)}. \quad (4)$$

In the square-lattice limit, the x - and y -axis branches are degenerate, whereas a finite rectangular deformation lifts this degeneracy and splits the original off- Γ BICs into two nonequivalent axis-pinned branches. Near the critical aspect ratio $R_{0,x}$, at which the x -axis A-BICs merge at the Γ point, expansion of $\alpha_x(R)$ and $\beta_x(R)$ gives

$$k_{BIC, x}^2 \approx C_x(R - R_{0,x}), \quad (5)$$

or equivalently $k_{BIC, x} \propto (R - R_{0,x})^{1/2}$, where C_x is an effective coefficient determined by the local variation of the far-field expansion coefficients with R . Similarly, we have $k_{BIC, y} \propto (R_{0,y} - R)^{1/2}$, indicating that when BICs on the k_x axis approach the Γ point, the A-BICs on the k_y axis move away from Γ point. This semianalytical picture explains the square-root evolution of the BIC position observed in Fig. 2(b) and clarifies the axis-pinned branch splitting induced by rectangular lattice engineering. This relation provides a practical estimate of the aspect ratio required to place an axis-pinned BIC at a target momentum within the validity range of the low-order expansion. This range corresponds approximately to $0.04 < |k_{BIC}a/2\pi| < 0.09$. A more detailed derivation can be found in Appendix A.

If the square lattice is replaced with a monoclinic lattice by introducing the included angle and fixing the area of the unit cell, these BICs experience a merging process along different paths in the momentum space. Figure 3(a) presents the magnetic field distribution of the eigenmode in a PCS with a monoclinic lattice, which clearly demonstrates the twisted field distribution of the BIC mode due to the lattice symmetry. In momentum space, we analyze the dependence of the Q-factor on the wave vector $\mathbf{k}$ along two semidiagonal

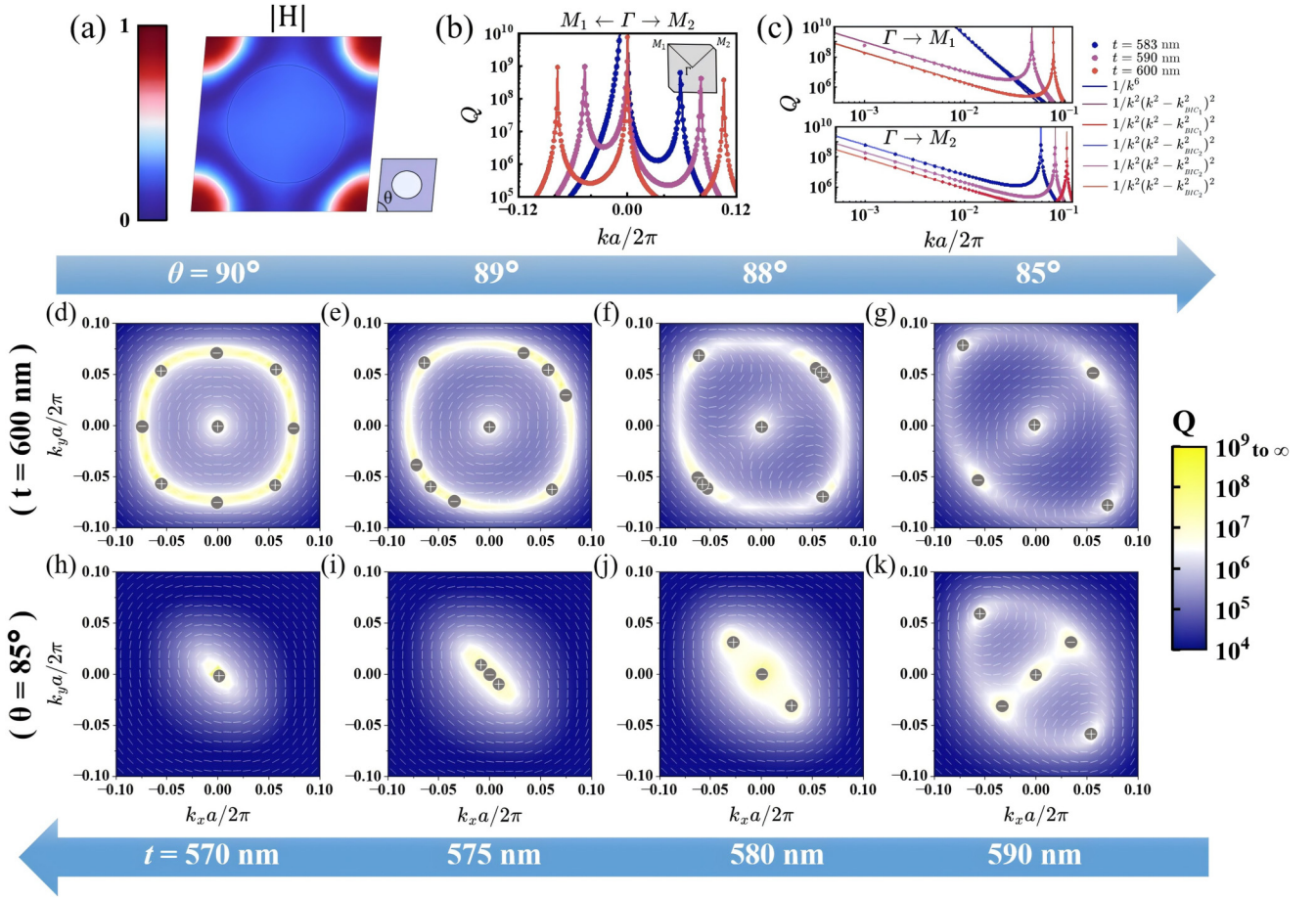


FIG. 3. BIC evolution in monoclinic lattice PCS under lattice angle and thickness engineering. (a) Eigenfield distribution of Hz component in the monoclinic lattice. (b) Q-factor distribution along the two semidiagonal directions in momentum space. (c) Fitting curves of the Q-factor distribution along the two semidiagonal directions. [(d)–(g)] Evolution of BICs in momentum space as the lattice angle θ decreases from 90° to 85° at a fixed thickness $t = 600$ nm. [(h)–(k)] Evolution of BICs merging to the Γ point in momentum space as the thickness t is tuned from 570 to 590 nm at a fixed lattice angle $\theta = 85^\circ$.

directions ($M_1 \leftarrow \Gamma \rightarrow M_2$), as shown in Fig. 3(b). We further fit the Q-factor with the form $1/[k^2(k^2 - k_{\text{BIC}}^2)^2]$ [Fig. 3(c)], which verifies the dependence of BIC radiation loss on the wave vector and shows excellent agreement with the theoretical prediction.

To study the effect of the included angle on the BICs in the momentum space, we fix the thickness $t = 600$ nm and gradually decrease the included angle θ . The relevant results are shown in Figs. 3(d)–3(g). At $\theta = 90^\circ$, there exists an SP-BIC with a topological charge $q = +1$ at the Γ point, accompanied by multiple A-BICs with $q = \pm 1$ distributed along the high-symmetry lines. In contrast to rectangular deformation, monoclinic shear removes the mirror symmetries with respect to the x and y axes, thereby releasing the BICs from their axis-pinned trajectories. Defining the shear parameter as $\sigma = \pi/2 - \theta$, the far-field radiation vector near the rectangular-lattice limit can be expressed as

$$\mathbf{c}(\mathbf{k}, \sigma) = \begin{pmatrix} \alpha_x & \sigma\mu_x \\ \sigma\mu_y & \alpha_y \end{pmatrix} \begin{pmatrix} k_x \\ k_y \end{pmatrix} + \mathbf{c}^{(3)}(\mathbf{k}, \sigma) + \dots \quad (6)$$

At $\sigma = 0$, the linear coupling matrix is diagonal, consistent with the axis-pinned BIC branches in the rectangular lattice. Monoclinic shear introduces the off-diagonal terms $\sigma\mu_x$ and

$\sigma\mu_y$, which couple the orthogonal momentum components and allow the BICs to leave the principal axes. For a BIC initially located on the k_x axis, perturbation analysis gives

$$\frac{k_y}{k_x} = C\sigma + O(\sigma^2), \quad (7)$$

where C is determined by the far-field expansion coefficients. This leading-order relation agrees well with the numerical results, while the complete derivation is provided in Appendix B. As a result, the A-BICs with $q = -1$ located on the horizontal and vertical axes gradually approach the A-BICs with $q = +1$ on the antidiagonals and eventually merge into two BICs with $q = -1$ on the antidiagonals. This process reveals the crucial role played by the included angle of the monoclinic lattice in engineering BICs.

These BICs can be further engineered to merge along the diagonal and antidiagonal by tuning the thickness, as confirmed in Figs. 3(h)–3(k). As the thickness decreases from $t = 600$ to 580 nm, the A-BICs along the diagonals approach the Γ point and ultimately merge with the BIC at Γ point, forming a single super BIC with $q = -1$. Further reducing the thickness to $t = 570$ nm leads to the merging of the two A-BICs with $q = +1$ along the antidiagonals and the BIC

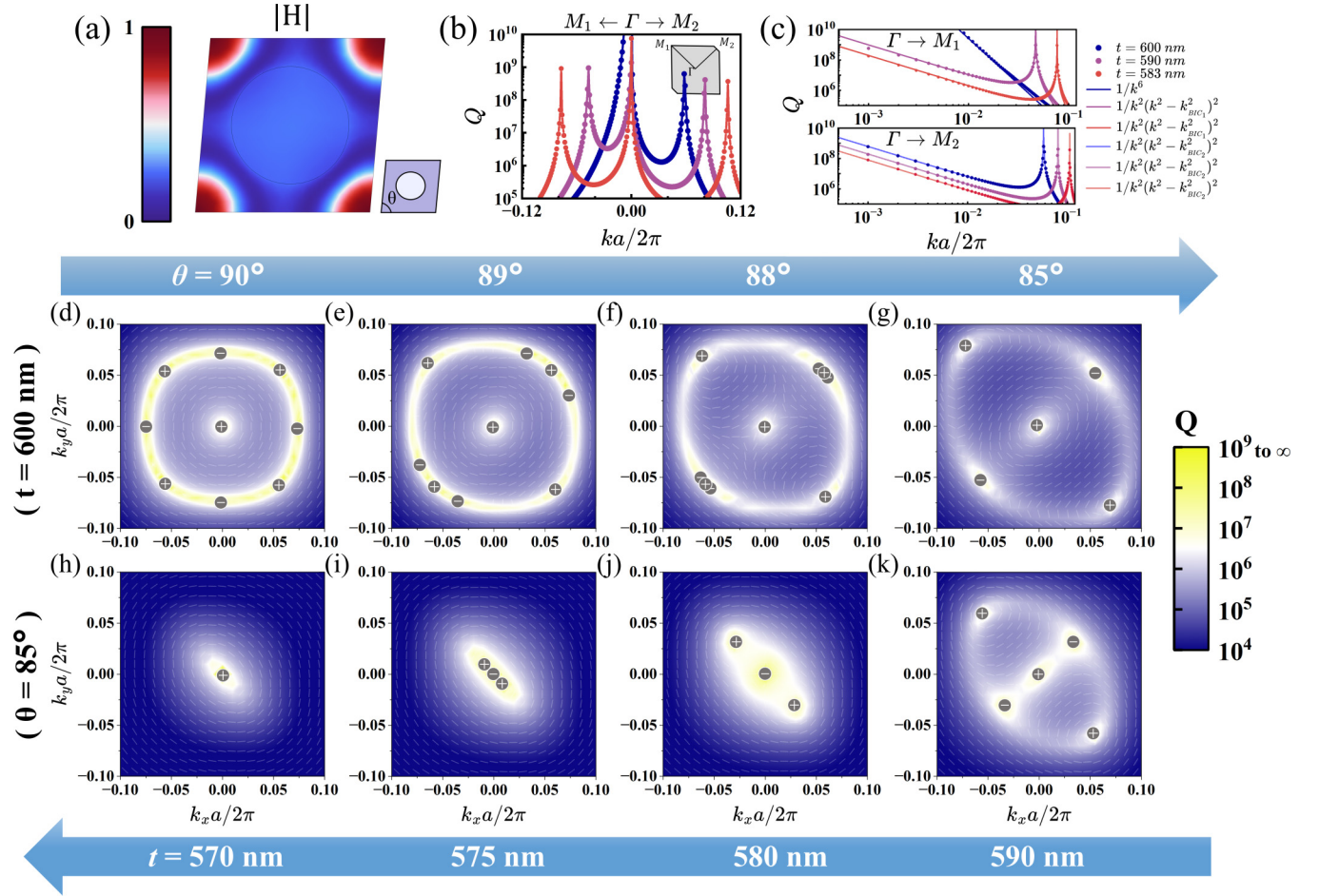


FIG. 4. BIC evolution and C-point formation in a symmetry-broken monoclinic lattice PCS. (a) Eigenfield distribution of Hz component in the monoclinic lattice with a crescent-shaped hole. (b) Ellipticity (ρ) and Q-factor obtained by scanning along the gray dashed line in (g), with their minimum values in the inset. [(c)–(e)] Q-factor mapping in momentum space at thicknesses $t = 600, 590$, and 580 nm, respectively. [(f)–(h)] Corresponding ellipticity(ρ) mapping in momentum space for the thicknesses in (c)–(e).

at the Γ point into a single BIC with $q = +1$. The unique merging process indicates that anisotropic merging of BICs can be achieved by the synergistic regulation of thickness and other structural parameters in the monoclinic lattice.

It is well known that breaking symmetry can lead to the splitting of BICs with $q = +1$ or -1 into two chiral QBICs with half topological charges $q = +1/2$ or $q = -1/2$. To induce a chiral QBIC, one can break the C_2 symmetry of the monoclinic lattice. For example, we fix the lattice included angle as $\theta = 85^\circ$ and create a crescent-shaped air hole by excavating a small hole with a radius of 80 nm, as shown in Fig. 4. The evolution of ellipticity during the transition from a circular hole to a crescent-shaped hole can be found in Fig. S1. Figure 4(a) presents the magnetic field distribution of QBIC in a PCS with crescent-shaped air holes. For $t = 600$ nm, it can be seen from Figs. 4(c) and 4(f) that the BICs with integer topological charges are split into multiple C-points with half topological charges $q = \pm 1/2$ as the symmetry is further broken. As the thickness is reduced to $t = 590$ nm [Figs. 4(d) and 4(g)], these C-points gradually approach the Γ point. Remarkably, an extended region of near-circularly polarized high-Q states is observed along the selected momentum-space path in Fig. 4(b) by calculating the ellipticity ρ along the

gray dashed line in Fig. 4(g). This provides a feasible route for obtaining high-Q states with high ellipticity over a finite momentum-space range. The momentum-space overlap between the high-Q and high-ellipticity regions is further illustrated in Fig. S2 of SM [63]. After reducing the thickness to $t = 580$ nm, the three C-points along the gray dashed line merge, generating C points with topological charges of $+1/2$ and $-1/2$, respectively.

Note that these C-points can be further manipulated by rotating the crescent-shaped hole around the lattice center. As clearly shown in Fig. 5(a), when the small hole is rotated to $\varphi = 90^\circ$, the distribution of C-points in the momentum space becomes mirror-symmetric to that at $\varphi = 0^\circ$. When $\varphi = 180^\circ$, the distribution returns to the exact same state as at $\varphi = 0^\circ$. By analyzing the evolution process from $\varphi = 0^\circ$ to 90° in detail, we find that within the range of $\varphi = 10^\circ$ to 20° , the left-hand circularly polarized (LCP) and right-hand circularly polarized (RCP) states with topological charges $q = +1/2$ and $q = -1/2$ first approach each other and then separate [Fig. 5(b)]. A similar behavior occurs within the range of $\varphi = 70^\circ$ to 80° , but with an overall mirror-reversed pattern. During the transition from $\varphi = 40^\circ$ to 50° , the RCP and LCP states with $q = -1/2$ undergo a significant displacement. At

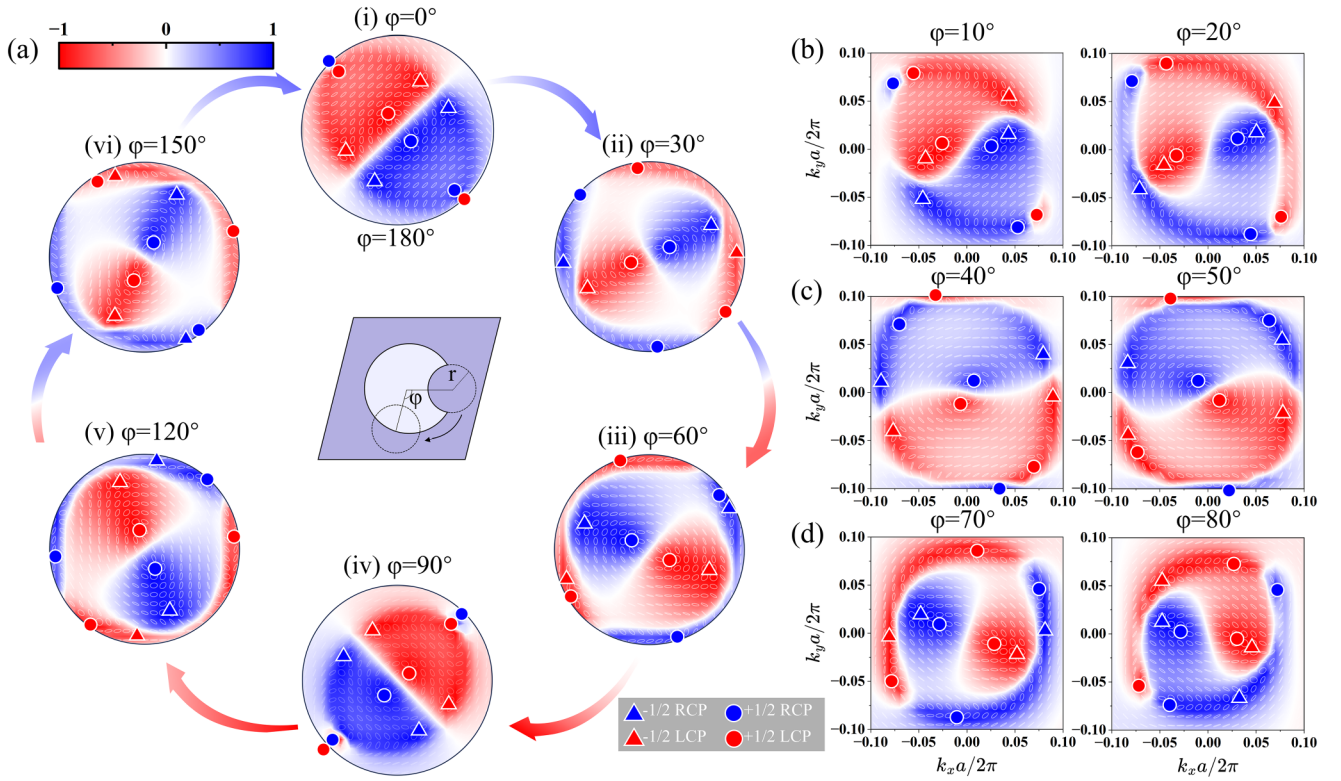


FIG. 5. Rotation-controlled rearrangement of C-points in a monoclinic PCS with crescent-shaped holes. (a) Evolution of ellipticity in momentum space as the small hole rotates 180° around the lattice center, with rotation angles $\varphi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ$, and 150° . [(b)–(d)] Detailed supplementary views of ellipticity in momentum space at additional rotation angles $\varphi = 10^\circ, 20^\circ, 40^\circ, 50^\circ, 70^\circ$, and 80° .

$\varphi = 60^\circ$, they exhibit a merging-like behavior with the RCP and LCP states with $q = +1/2$, respectively. These results demonstrate that by changing the orientation of the crescent-shaped hole, we can effectively control the distribution of C-points in momentum space, providing a new degree of freedom for the precise manipulation of chiral optical responses.

Finally, we note that C_{4v} symmetry can also be reduced to C_{2v} symmetry by replacing circular holes with elliptical holes while the square lattice of the PCS is preserved. Figure 6 shows the BIC evolution under such a unit-cell geometric engineering in a fixed square lattice. Similar to lattice engineering, breaking C_{4v} symmetry via elliptical perturbation (dR) or rotation ($d\varphi$) can also drive BIC merging. We also observe similar phenomena in a PCS with a rectangular hole, as shown in Fig. S3 of SM [63]. The sidewall-taper tests in Fig. S5 of SM [63] show comparable sensitivity for the lattice- and super-atom-engineered structures. However, the elliptical-hole design is additionally affected by eccentricity deviations, whereas the lattice-engineered structure uses circular holes and therefore avoids this additional shape-error channel. The practical advantage of lattice engineering thus lies in reducing the number of geometrical parameters that require precise fabrication control.

IV. CONCLUSION

In summary, we realize the flexible manipulation of BICs in a silicon PCS via lattice engineering, achieving structural evolution from square lattices to rectangular and monoclinic lattices with conserved unit cell area. Tuning the aspect ratio

of the rectangular lattice lifts the degeneracy between the orthogonal BIC branches while preserving the axial mirror constraints, thereby enabling their axis-pinned compression and merging in momentum space. Near the merging point, the squared BIC position k_{BIC}^2 varies linearly with the aspect-ratio detuning, providing a direct relation between the lattice geometry and the BIC position. Further modulating the thickness allows for the merging of three BICs along k_y axis into a single one at Γ point. For monoclinic lattices, reducing the included angle removes the axial constraints and induces anisotropic off-axis trajectories and merging of BICs, while complementary thickness tuning further drives the merged BICs toward the Γ point. By designing crescent-shaped air holes to break the in-plane C_2 symmetry of monoclinic lattices, BICs carrying integer topological charge split into multiple C-points with half topological charges. Additionally, we construct extended high-ellipticity regions in the momentum space by tuning the thickness. Rotating the crescent-shaped holes triggers dynamic displacement and rearrangement of C-points around the Γ point. Finally, we show that BICs can be engineered by replacing the circular holes within the unit cell with elliptical holes. Overall, this work establishes a symmetry-guided framework in which lattice symmetry constrains the allowed BIC trajectories, continuous lattice deformation controls their momentum-space positions, and slab thickness provides a complementary degree of freedom for completing their merging. These results deepen the understanding of BIC evolution in low-symmetry lattices and provide a systematic route for engineering BICs and polarization singularities in photonic structures.

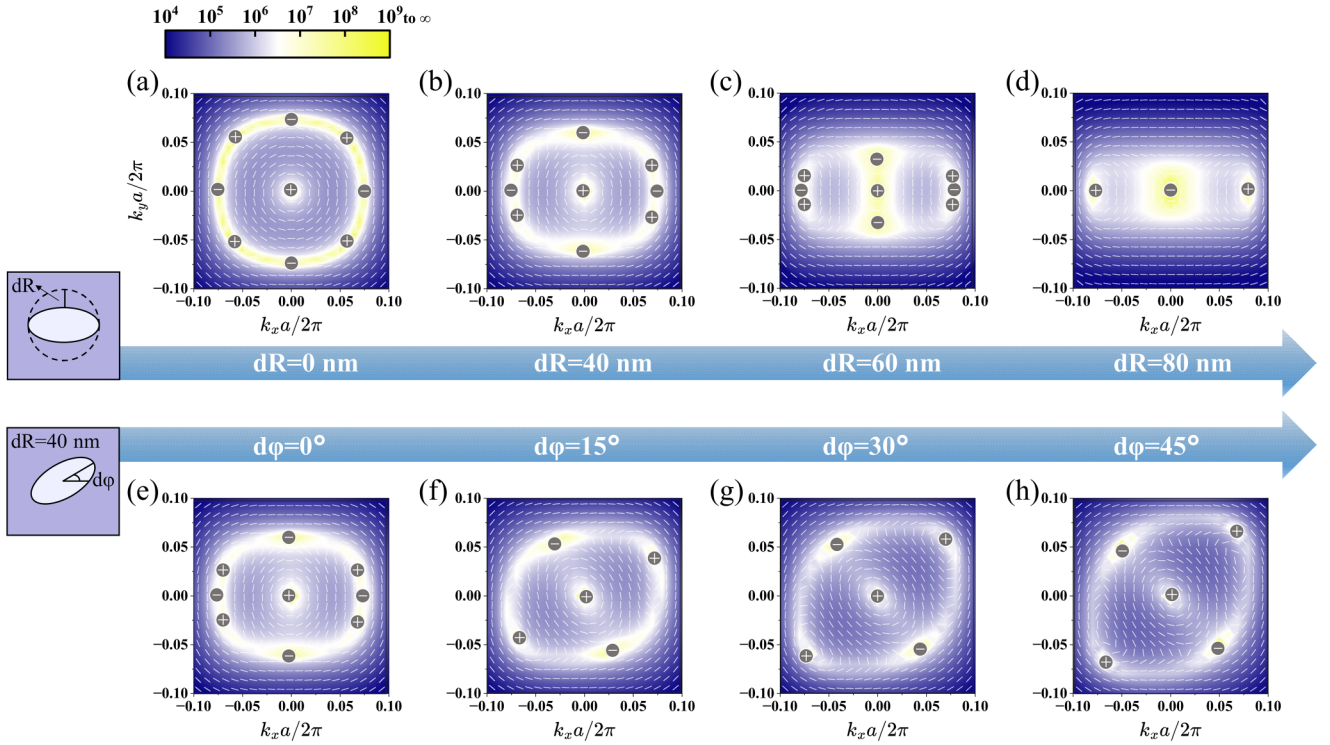


FIG. 6. Manipulating the BICs in momentum space by geometric engineering with the central circular hole. [(a)–(d)] Momentum-space evolution of BICs in a fixed square lattice as the scattering element is continuously transformed from a circular hole to an ellipse. [(e)–(h)] Influence of the rotation angle $d\phi$ of the elliptical hole on the coordinates of accidental BICs with dR fixed at 40 nm.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: SEMIANALYTICAL THEORY FOR AXIS-PINNED BIC BRANCH SPLITTING IN RECTANGULAR LATTICES

In this appendix, we develop a perturbation theory for the rectangular-lattice stage of the BIC evolution. Our goal is to describe how the square-lattice degeneracy is lifted into two inequivalent axis-pinned off- Γ branches.

The basic idea is to treat a BIC as a zero of the far-field radiation vector $\mathbf{c}(\mathbf{k}, R) = (c_x, c_y)$, where $\mathbf{k} = (k_x, k_y)$ is the

in-plane Bloch wave vector and R denotes the lattice deformation parameter [32,43,64,65]. The BIC condition is therefore

$$c_x(\mathbf{k}, R) = 0, \quad (\text{A1})$$

$$c_y(\mathbf{k}, R) = 0. \quad (\text{A2})$$

For the rectangular lattice, the structure preserves mirror symmetries with respect to the x and y axes. As a result, the far-field radiation amplitudes near Γ can be expanded as

$$c_x = k_x [\alpha_x(R) + \beta_x(R)k_x^2 + \gamma_x(R)k_y^2 + \dots], \quad (\text{A3})$$

$$c_y = k_y [\alpha_y(R) + \beta_y(R)k_y^2 + \gamma_y(R)k_x^2 + \dots]. \quad (\text{A4})$$

Here, $\alpha_x, \alpha_y, \beta_x, \beta_y, \gamma_x, \gamma_y$ are effective coefficients depending on the lattice deformation R .

On the k_x axis ($k_y = 0$), one has

$$c_y = 0, \quad c_x = k_x (\alpha_x(R) + \beta_x(R)k_x^2 + \dots). \quad (\text{A5})$$

The nonzero off- Γ BICs satisfy

$$\alpha_x(R) + \beta_x(R)k_x^2 = 0, \quad (\text{A6})$$

which yields

$$k_{\text{BIC},x}^2 = -\frac{\alpha_x(R)}{\beta_x(R)}. \quad (\text{A7})$$

Similarly, on the k_y axis ($k_x = 0$),

$$k_{\text{BIC},y}^2 = -\frac{\alpha_y(R)}{\beta_y(R)}. \quad (\text{A8})$$

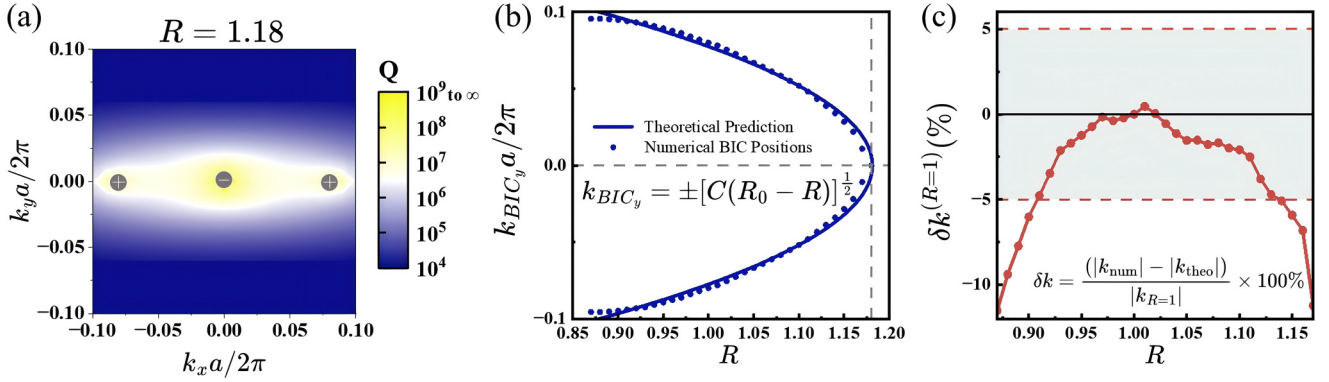


FIG. 7. Semianalytical description of the k_y -axis BIC evolution in the rectangular lattice. (a) Momentum-space Q-factor distribution at $R = 1.18$, showing the vertical compression of the k_y -axis BIC branch toward the Γ point. (b) Evolution of the k_y -axis BIC positions as a function of the aspect ratio R . The symbols denote numerically extracted BIC positions, while the solid curve shows the semianalytical prediction. The dashed vertical line marks the critical aspect ratio R_0 at which the two off- Γ BICs merge at the Γ point. (c) Relative deviation between the numerical and semianalytical BIC positions, defined as $\delta k = (|k_{\text{num}}| - |k_{\text{theo}}|)/|k_{R=1}| \times 100\%$. The red dashed lines indicate deviations of $\pm 5\%$.

In the square-lattice limit $R = 1$, the x and y directions are equivalent, and therefore

$$\alpha_x(1) = \alpha_y(1) = \alpha_0, \quad \beta_x(1) = \beta_y(1) = \beta_0. \quad (\text{A9})$$

Accordingly,

$$k_{BIC,x}^2 = k_{BIC,y}^2 = -\frac{\alpha_0}{\beta_0}. \quad (\text{A10})$$

For $R \neq 1$, this degeneracy is lifted. Since exchanging the x and y directions is equivalent to sending $R \rightarrow 1/R$, the coefficients satisfy

$$\alpha_y(R) = \alpha_x(1/R), \quad \beta_y(R) = \beta_x(1/R). \quad (\text{A11})$$

Expanding around the square-lattice point $R = 1$, we have

$$\alpha_x(R) = \alpha_0 + a_1(R - 1) + a_2(R - 1)^2 + \dots, \quad (\text{A12a})$$

$$\alpha_y(R) = \alpha_0 - \tilde{a}_1(R - 1) + \tilde{a}_2(R - 1)^2 + \dots, \quad (\text{A12b})$$

$$\beta_x(R) = \beta_0 + b_1(R - 1) + b_2(R - 1)^2 + \dots, \quad (\text{A12c})$$

$$\beta_y(R) = \beta_0 - \tilde{b}_1(R - 1) + \tilde{b}_2(R - 1)^2 + \dots \quad (\text{A12d})$$

The equalities of $a_1 = \tilde{a}_1$ and $b_1 = \tilde{b}_1$ are not additional assumptions, but follow directly from the exchange symmetry at $R = 1$. Indeed, writing $R = 1 + \delta$ with $|\delta| \ll 1$, we have

$$\frac{1}{R} = \frac{1}{1 + \delta} = 1 - \delta + \delta^2 + O(\delta^3). \quad (\text{A13})$$

Substituting this into the expansion for $\alpha_x(1/R)$ gives

$$\alpha_x(1/R) = \alpha_0 - a_1\delta + (a_1 + a_2)\delta^2 + \dots \quad (\text{A14})$$

Comparing this with the expansion of $\alpha_y(R)$, we immediately find

$$\tilde{a}_1 = a_1. \quad (\text{A15})$$

By the same argument,

$$\tilde{b}_1 = b_1. \quad (\text{A16})$$

Substituting these expressions into the position formula for the x -axis branch gives

$$k_{BIC,x}^2 = -\frac{\alpha_0 + a_1(R - 1)}{\beta_0 + b_1(R - 1)}. \quad (\text{A17})$$

Expanding the above expression to first order in $(R - 1)$, we obtain

$$k_{BIC,x}^2 \approx -\frac{\alpha_0}{\beta_0} - \frac{a_1\beta_0 - \alpha_0b_1}{\beta_0^2}(R - 1). \quad (\text{A18})$$

Similarly, for the y -axis branch:

$$k_{BIC,y}^2 = -\frac{\alpha_0 - a_1(R - 1)}{\beta_0 - b_1(R - 1)} \approx -\frac{\alpha_0}{\beta_0} + \frac{a_1\beta_0 - \alpha_0b_1}{\beta_0^2}(R - 1). \quad (\text{A19})$$

We define the initial squared displacement $k_{BIC_0}^2$ and the splitting coefficient C as

$$k_{BIC_0}^2 \equiv -\frac{\alpha_0}{\beta_0}, \quad C \equiv \frac{a_1\beta_0 - \alpha_0b_1}{\beta_0^2}. \quad (\text{A20})$$

The evolution of the two branches reduces to the following elegant linear forms:

$$k_{BIC,x}^2 \approx k_{BIC_0}^2 - C(R - 1), \quad (\text{A21})$$

$$k_{BIC,y}^2 \approx k_{BIC_0}^2 + C(R - 1). \quad (\text{A22})$$

The corresponding compact form quoted in the main text follows directly from the above first-order expansion.

$$k_{BIC,x} \approx \pm[-C(R - R_{0,x})]^{1/2}, \quad (\text{A23})$$

$$k_{BIC,y} \approx \pm[C(R_{0,y} - R)]^{1/2}. \quad (\text{A24})$$

The corresponding numerical results and semianalytical prediction are shown in Fig. 7.

APPENDIX B: SEMIANALYTICAL THEORY FOR SYMMETRY UNPINNING OF BIC BRANCHES IN MONOCLINIC LATTICES

In this appendix, we extend the above rectangular-lattice theory to the monoclinic case. In contrast to the rectangular lattice, the x and y axes in a monoclinic lattice are no longer mirror-symmetry axes. Consequently, the axial pinning of the BIC branches is removed, and off- Γ BICs are allowed to leave the coordinate axes and evolve into genuinely off-axis branches. Assuming the system preserves a global C_2 symmetry, the radiation field vector $\mathbf{c}(\mathbf{k})$ remains an odd function of $\mathbf{k}$, but linear mixing between orthogonal momentum directions is now permitted.

Therefore the lowest-order natural model for the monoclinic lattice should no longer assume strict axial separation. It is most accurately written as:

$$\begin{pmatrix} c_x \\ c_y \end{pmatrix} = M(\sigma) \begin{pmatrix} k_x \\ k_y \end{pmatrix} + \begin{pmatrix} N_x^{(3)}(k_x, k_y; \sigma) \\ N_y^{(3)}(k_x, k_y; \sigma) \end{pmatrix} + \dots \quad (\text{B1})$$

Here, σ represents the monoclinic shear parameter (e.g., the lattice angle deviation from 90°), $M(\sigma)$ is the linear term matrix, and $N^{(3)}$ encapsulates all allowed third-order terms.

In the rectangular lattice limit ($\sigma=0$), the linear matrix is strictly diagonal:

$$M(0) = \begin{pmatrix} \alpha_x & 0 \\ 0 & \alpha_y \end{pmatrix}. \quad (\text{B2})$$

However, in the monoclinic phase, off-diagonal terms immediately emerge at the lowest order:

$$M(\sigma) = \begin{pmatrix} \alpha_x & \sigma\mu_x \\ \sigma\mu_y & \alpha_y \end{pmatrix} + O(\sigma^2). \quad (\text{B3})$$

The parameters μ_x and μ_y are the linear cross-coupling coefficients introduced by the monoclinic shear. Their nonzero presence signifies that c_x is no longer solely dependent on k_x , and c_y is no longer solely dependent on k_y . This lifts the symmetry pinning of the BICs, marking the key theoretical shift in the monoclinic phase.

To capture the existence of off- Γ BICs, the linear terms must compete with third-order terms. The minimal practical model is constructed as

$$c_x = \alpha_x k_x + \sigma\mu_x k_y + \beta_x k_x^3 + \gamma_x k_x k_y^2 + \sigma(u_x k_x^2 k_y + v_x k_y^3) + \dots, \quad (\text{B4a})$$

$$c_y = \alpha_y k_y + \sigma\mu_y k_x + \beta_y k_y^3 + \gamma_y k_y k_x^2 + \sigma(u_y k_y k_x^2 + v_y k_x^3) + \dots \quad (\text{B4b})$$

Here $\alpha_{x,y}$ control the proximity of the branches to Γ , $\beta_{x,y}$ and $\gamma_{x,y}$ describe the longitudinal and transverse cubic curvatures, and $\mu_{x,y}$ denote the linear mixing terms opened by the loss of mirror symmetry. The $u_{x,y}$ and $v_{x,y}$ terms are higher-order monoclinic corrections. To leading order, the off-axis motion is controlled by μ_x and μ_y .

To analytically describe these dynamics, we apply a perturbation approach starting from the axial BICs in the rectangular lattice ($\sigma=0$). Assume a pair of BICs is pinned on the x axis

at

$$(k_x, k_y) = (\pm k_0, 0), \quad k_0^2 = -\frac{\alpha_x}{\beta_x}. \quad (\text{B5})$$

Introducing a small monoclinic shear ($\sigma \neq 0$), we define the new BIC coordinates as

$$k_x = k_0 + \sigma\delta k_x + O(\sigma^2), \quad (\text{B6a})$$

$$k_y = \sigma\delta k_y + O(\sigma^2). \quad (\text{B6b})$$

Substituting these into the zero-field conditions ($c_x=0, c_y=0$), we first evaluate the transverse evolution ($c_y=0$) up to $O(\sigma)$:

$$0 = \alpha_y k_y + \sigma\mu_y k_x + \gamma_y k_y k_x^2 + \dots \quad (\text{B7})$$

Substituting $k_x = k_0$ and $k_y = \sigma\delta k_y$ yields

$$0 = \sigma\delta k_y (\alpha_y + \gamma_y k_0^2) + \sigma\mu_y k_0. \quad (\text{B8})$$

Solving for the first-order transverse correction:

$$\delta k_y = -\frac{\mu_y k_0}{\alpha_y + \gamma_y k_0^2}. \quad (\text{B9})$$

Thus

$$k_y = -\sigma \frac{\mu_y k_0}{\alpha_y + \gamma_y k_0^2} + O(\sigma^2). \quad (\text{B10})$$

This critical result reveals that upon the introduction of monoclinic deformation, the BIC originally pinned on the x axis immediately deviates from the coordinate axis at linear order ($k_y \propto \sigma$).

Evaluating the longitudinal evolution ($c_x=0$) up to $O(\sigma)$:

$$0 = \alpha_x k_x + \beta_x k_x^3 + \dots \quad (\text{B11})$$

Substituting $k_x = k_0 + \sigma\delta k_x$ and utilizing the equilibrium condition $\alpha_x k_0 + \beta_x k_0^3 = 0$:

$$0 = (\alpha_x + 3\beta_x k_0^2)\delta k_x. \quad (\text{B12})$$

Since $k_0^2 = -\alpha_x/\beta_x$, the coefficient becomes

$$\alpha_x + 3\beta_x k_0^2 = \alpha_x - 3\alpha_x = -2\alpha_x \neq 0. \quad (\text{B13})$$

Consequently,

$$\delta k_x = 0, \quad (\text{B14})$$

which implies

$$k_x = k_0 + O(\sigma^2). \quad (\text{B15})$$

This demonstrates that under a small monoclinic shear, the transverse shift (k_y) is linear, whereas the longitudinal position (k_x) correction is strictly of the second order. Therefore the BIC trajectory initially manifests as remaining nearly stationary along the original axis while rapidly moving perpendicularly.

The initial deflection rate of the original x -axis branch is given by

$$\frac{k_y}{k_x} \approx -\sigma \frac{\mu_y}{\alpha_y + \gamma_y k_0^2}. \quad (\text{B16})$$

The corresponding angular evolution of the off-axis BIC branches is shown in Fig. 8.

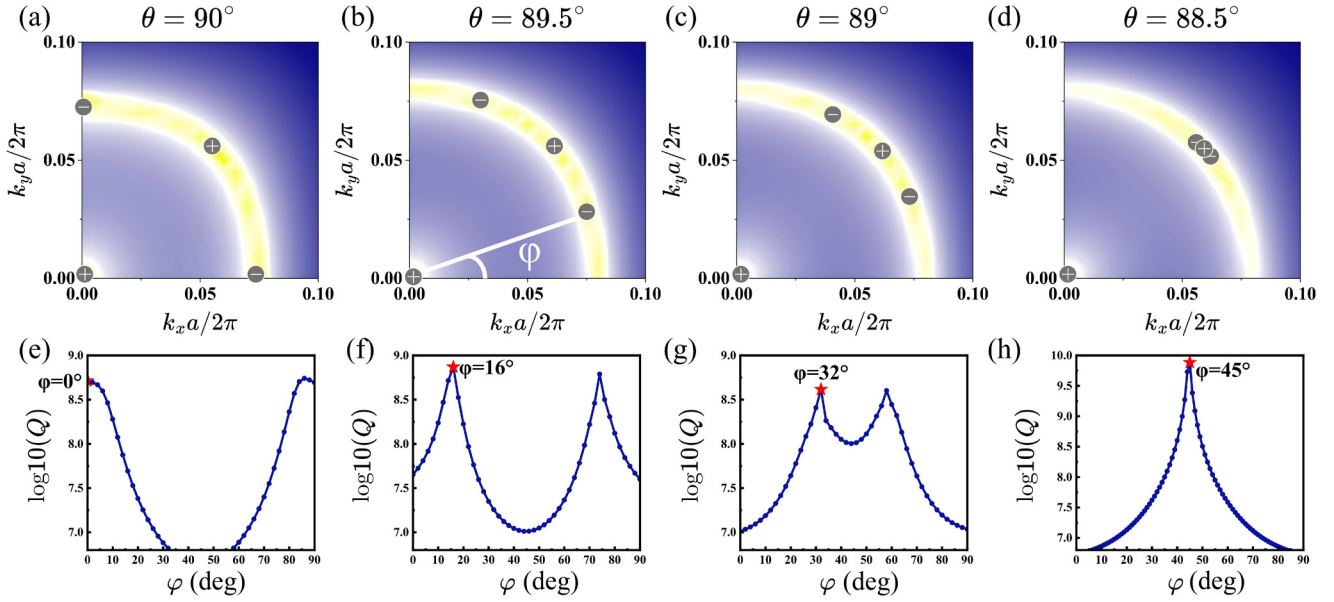


FIG. 8. Angular evolution of off-axis BIC branches in the monoclinic lattice. [(a)–(d)] Momentum-space Q-factor maps for lattice angles $\theta = 90^\circ$ (a), 89.5° (b), 89° (c), and 88.5° (d), respectively. As the lattice angle is reduced from the square-lattice limit, the BICs initially pinned on the k_x and k_y axes gradually leave the original symmetry axes and evolve toward the diagonal direction in momentum space. [(e)–(h)] Q-factor profiles obtained by scanning along a circle centered at Γ with radius k_{BIC} , corresponding to (a)–(d). The extracted peak angles are $\varphi = 0^\circ$, 16° , 32° , and $\varphi = 45^\circ$, indicating an approximately linear increase of the deflection angle with the lattice-angle deviation from the square-lattice limit, which is in good agreement with Eq. (B16). When $\theta = 88.5^\circ$, φ should have been 48° according to the linear dependence, but a locking of the BIC trajectory near the diagonal direction emerges as Eq. (B20) predicts.

This establishes a robust direction selection law: the initial off-axis trajectory is no longer dictated by the previous high-symmetry axes, but is jointly determined by the monoclinic mixing coefficient μ_y and the transverse stiffness $(\alpha_y + \gamma_y k_0^2)$.

The above result only gives the initial deflection for small σ . As σ increases further, the dominant direction is no longer the coordinate axes but the natural principal axis of the full zero-point equation.

From the linear part, this direction is determined by the eigenvectors of the matrix

$$M(\sigma) = \begin{pmatrix} \alpha_x & \sigma\mu_x \\ \sigma\mu_y & \alpha_y \end{pmatrix}. \quad (\text{B17})$$

Writing the eigenvector as $(1, r)^T$ with $r = k_y/k_x$, the condition $M(\sigma)(1, r)^T = \lambda(1, r)^T$ yields

$$\sigma\mu_x r^2 + (\alpha_x - \alpha_y)r - \sigma\mu_y = 0. \quad (\text{B18})$$

In the square lattice, the x and y directions are equivalent; after introducing a strong perturbation σ , for instance $\theta = 85^\circ$, we have

$$\alpha_x \approx \alpha_y, \quad \mu_x \approx \mu_y, \quad \sigma \neq 0, \quad (\text{B19})$$

then the result above becomes

$$\sigma\mu(r^2 - 1) \approx 0, \quad (\text{B20})$$

so $r \approx \pm 1$, $\varphi \approx 45^\circ$ or 135° , which is in line with Fig. 3 in the main text.

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