

Intrinsic chiral optical vortex emission from the interactions between free electrons with bound states in the continuum

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We present an approach for free-electron-driven optical vortex emission through interaction with the quasi-bound states in the continuum (quasi-BICs). Based on a unified framework for free electron-nanophotonic interaction and time domain simulations, we show that the free electron beam can efficiently excite the quasi-BIC under the phase-matching condition. The intrinsic k -space polarization anisotropy associated with the quasi-BIC imprints a geometric phase onto the emission, and thus generates an intrinsic optical vortex. We then reveal a link between the topological charge of the quasi-BIC and the emitted optical vortex by analyzing the far-field polarization structure and phase distribution. This mechanism offers a promising approach to creating nanoscale electron-beam-driven structured light sources without the need for complex chiral nanostructures, thereby advancing the interdisciplinary study of free-electron optics and nanophotonics.

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I. INTRODUCTION

Recently, the interaction between free electrons and nanophotonic structures has attracted great interest because it provides a fertile ground for exploring fundamental light-matter physics and developing electron-driven light sources [1,2]. This manifests itself in both stimulated [3–6] and spontaneous processes [7–10]. Various types of spontaneous processes, such as Cherenkov radiation, transition radiation, and Smith-Purcell radiation (SPR), offer a promising method for generating ultrabroadband light, ranging from the infrared to the ultraviolet region. The radiation produced is inherently phase-locked to the source electron, thus termed coherent cathodoluminescence (CL). Integrating nanostructures facilitates miniaturization and enables enhanced [8,11,12], versatile control over emission characteristics, such as polarization [13], focus [14–16], and emission angle [17,18].

The ability to harness light across all its degrees of freedom and dimensions is also developing rapidly. Looking into the future, the next step is to generate free-electron radiation with controlled spin and orbital angular momentum of CL [19]. Electron-beam-driven light sources have shown promise in

generating structured light, including optical vortices [20,21] and collimated light [22,23]. In prominent demonstrations of electron-beam optical vortex emission, the mechanism typically involves electron interaction with chiral nanostructures to excite chiral surface plasmon polaritons. Consequently, the optical vortex depends on the chirality of the nanostructures and is therefore extrinsic. Recent advances in optically excited bound states in the continuum (BICs) have enabled optical vortex generation in momentum space, without the need for structures with real-space chirality or geometric centers [24,25]. As a polarization singularity in momentum space, a BIC exhibits a unique confinement property in the vertical direction with a diverging quality (Q) factor. Nevertheless, an ideal BIC decouples from free space modes. In reality, a quasi-BIC (quasi-bound state in the continuum) that arises from the structural imperfection, finite-size effect, and material absorption loss is more suitable for application in generating optical vortices with a well-defined topological charge [26–30]. However, the optical excitation efficiency of the quasi-BIC remains inherently low due to the weak coupling. Here, the free-electron source emerges as a powerful alternative. Coupling sheetlike free electrons with a BIC has been demonstrated to significantly enhance spontaneous emission [8,12], making it an attractive way to generate optical vortices with a controllable intrinsic topological charge.

In this article, we show that the intrinsic optical vortex emission can be realized through the interaction of pointlike free electrons with the quasi-BIC on an easily fabricated photonic crystal slab (PCS). Starting with a unified theoretical framework of free-electron radiation in arbitrary nanophotonic structures, we demonstrate that the phase-matched

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electron beams with maximal mode-electron overlap can efficiently excite BICs. Guided by parameters approximated from above, we further perform finite-difference time domain (FDTD) simulations to model the interaction between free electrons and quasi-BICs supported by finite-size PCS. The calculated radiative power and the electron energy loss spectrum (EELS) enable us to refine and validate the excitation parameters. Then we analyze the far-field intensity and polarization distributions, which reveal the efficient formation of a polarization vortex in momentum space. When the far-field emission is projected onto a circular polarization basis, the induced Pancharatnam-Berry (PB) phase generates an optical vortex in both real and k -spaces whose topological charge directly links to that of the quasi-BIC. Quasi-BICs excited by a free-electron beam suggest an alternative mechanism for achieving vortex lasing at the nanoscale.

II. STRUCTURAL DESIGN AND THEORETICAL FRAMEWORK

In an infinite PCS with C_{4v} symmetry and periodicity p , the electric field of an eigenmode can be written as $\mathbf{E}_{\mathbf{k}}(\boldsymbol{\rho}) = e^{i\mathbf{k}\cdot\boldsymbol{\rho}} \mathbf{u}_{\mathbf{k}}(\boldsymbol{\rho})$, where $\mathbf{u}_{\mathbf{k}}(\boldsymbol{\rho})$ is a periodic function in both x and y directions. Here, $\boldsymbol{\rho} = x\hat{x} + y\hat{y}$ denotes the in-plane coordinates and $\mathbf{k} = k_x\hat{x} + k_y\hat{y}$ denotes the in-plane wave vector. For modes below the diffraction limit, the only allowed radiation channel is zero-order diffraction. The radiation amplitude through this channel is given by the vector $\mathbf{c}(\mathbf{k}) = \langle \mathbf{u}_{\mathbf{k}}(\boldsymbol{\rho}) \rangle$, representing the spatial average of $\mathbf{u}_{\mathbf{k}}(\boldsymbol{\rho})$ over a unit cell (indicated by angle brackets). This vector, $\mathbf{c}(\mathbf{k}) = c_x\hat{x} + c_y\hat{y}$, defines the k -space state of polarization (SOP) of the resonant mode at wave vector $\mathbf{k}$.

The BIC of an infinite PCS corresponds to a resonant mode that is completely decoupled from the propagating waves in free space, which results in an ill-defined SOP. Theoretical studies have shown that, in a system with time-reversal symmetry, the SOPs of resonant modes near a BIC are linearly polarized, with the differentiable polarization angle $\phi(\mathbf{k}) = \arg[c_x(\mathbf{k}) + ic_y(\mathbf{k})]$ rotating continuously around the BIC in k -space [26]. This allows us to define a winding number

$$q = \frac{1}{2\pi} \oint_C \mathbf{dk} \cdot \nabla_{\mathbf{k}} \phi(\mathbf{k}), \quad (1)$$

where C is a closed loop encircling the BIC in k -space. This winding number, also referred to as the topological charge of the BIC, underscores the topological protection inherent to BIC. The most common mechanism for BIC formation is the symmetry mismatch between its mode profile inside PCS and the external radiation continuum. It often appears at the high symmetry pointlike Γ point in k -space and is termed symmetry-protected BIC [31]. BICs have been used to generate the real-space optical vortex with optical pumping [25,32,33]. This method utilizes the topological vortexlike polarization in k -space surrounding the BIC; exciting BIC with near-normally incident, slightly convergent circularly polarized light couples nearby modes, which induces the PB phase and spin-orbit interactions necessary to form the vortex in the output beam.

To explore the feasibility of optical vortex emission from BICs that are excited by free electrons, we study the PCS

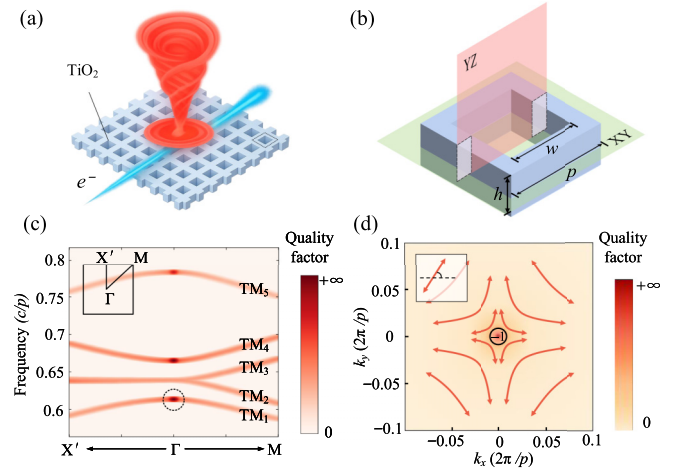


FIG. 1. Schematic and properties of the PCS supporting symmetry-protected Γ -BICs. (a) Illustration of optical vortex emission resulting from free-electron interaction with the BIC. (b) Unit cell of the PCS, w , h , and p denote the side length of the square air hole, slab thickness, and lattice constant, respectively. (c) Band structure of the infinite PCS for transverse magnetic (TM) modes with $w = 210$ nm, $h = 220$ nm, and $p = 340$ nm. Diverging quality factors at the Γ point in the TM_1 , TM_4 , and TM_5 bands signify the presence of BICs. (d) SOPs of the TM_1 mode near the Γ point, exhibiting a topological charge of -1 , and the inset shows the definition of the polarization angle $\phi(\mathbf{k})$. The band structure and SOP distribution are acquired using 3D finite element method by COMSOL.

structure with a freestanding TiO_2 film, as shown in Fig. 1(a). The unit cell consists of a square air hole etched into the TiO_2 film. The geometric parameters—air hole side length (w), slab thickness (h), and lattice constant (p)—are marked in Fig. 1(b). We calculate the band structure and SOPs by scanning the wave vector $\mathbf{k}$ throughout the first Brillouin zone. The calculation is performed using the finite element method (FEM) with the frequency-domain electromagnetic solver in the software COMSOL Multiphysics. Bloch boundary conditions are applied in both the x and y directions, while the perfect matched layers (PMLs) are applied in the z direction. One can find that the TM_1 , TM_4 , and TM_5 bands support BICs that are characterized by the diverging Q factors [Fig. 1(c)]. The SOP distribution of the TM_1 mode near the Γ point is depicted in Fig. 1(d), with a topological charge of -1 .

In nanophotonics, the interaction between free electrons and photonic quasiparticles can be described within a unified theoretical framework [2]. Here we consider a swift electron moving with a constant velocity $\mathbf{v} = v\hat{y}$ along the y axis (i.e., we ignore the quantum recoil correction). Its position at time t is given by $\mathbf{r}(t) = (x, vt, z)$. The associated current source density formulated in Gaussian units is $\mathbf{J}(\mathbf{r}, \omega) = -e\hat{y}\delta(x - x_0)\delta(z - z_0)e^{i\omega y/v}$, where e is the elementary charge, and x_0 and z_0 denote the position of the free electron in the XZ plane. The induced electric field is given by

$$\mathbf{E}^{\text{ind}}[\mathbf{r}(t), \omega] = -4\pi i\omega \int \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) \cdot \mathbf{J}(\mathbf{r}', \omega) d\mathbf{r}'. \quad (2)$$

The Green dyadic tensor $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega)$ satisfies the relation of $[\epsilon(\mathbf{r}, \omega) \frac{\omega^2}{c^2} - \nabla \times \nabla \times] \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \frac{1}{c^2} \delta(\mathbf{r} - \mathbf{r}') \mathbf{I}$, where $\epsilon(\mathbf{r}, \omega)$ is the dielectric function and $\mathbf{I}$ represents the 3×3 unit tensor. The Green dyadic tensor can be expanded in terms of the eigenmodes of the PCS,

$$\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \sum_m [\mathbf{E}_m(\mathbf{r}, \omega) \otimes \mathbf{E}_m^*(\mathbf{r}', \omega)] \cdot g(\omega, \omega_m). \quad (3)$$

$g(\omega, \omega_m) = (\omega^2 - \omega_m^2 - 2i\omega_m\gamma_m)^{-1}$ describes the spectral dependence, where ω_m is the resonant angular frequency and γ_m is the damping rate of the mode m . The damping rate γ_m determines the spectral linewidth of the resonance. The normalized eigenmodes $\mathbf{E}_m(\mathbf{r}, \omega)$ satisfy the following orthonormalized relation $\int_V \frac{1}{2\omega_m} \frac{d}{d\omega} (\epsilon(\mathbf{r}, \omega) \omega^2) \mathbf{E}_m(\mathbf{r}, \omega) \mathbf{E}_n^*(\mathbf{r}, \omega) dV = \delta_{mn}$. Finally, the EELS from a free electron interacting with nanophotonic quasiparticles can be written as

$$\begin{aligned} \Gamma_{\text{loss}}(\mathbf{R}_0, \omega) &= \frac{e}{\pi \hbar \omega} \int \text{Re}\{e^{-i\omega t} \mathbf{v} \cdot \mathbf{E}^{\text{ind}}[\mathbf{r}_e(t), \omega]\} dt \\ &= \frac{4e^2}{\hbar} \int dy dy' \text{Im}\{e^{i\omega(y-y')/v} \\ &\quad \times [-G_{yy}(\mathbf{R}_0, y, \mathbf{R}_0, y', \omega)]\} \\ &= -\frac{4e^2}{\hbar} \int dy dy' \text{Im}\{e^{i\omega(y-y')/v} \\ &\quad \times \sum_m E_{my}(y, \mathbf{R}_0, \omega) E_{my}^*(y', \mathbf{R}_0, \omega) g(\omega, \omega_m)\}, \end{aligned} \quad (4)$$

where $E_{my} = \hat{\mathbf{y}} \cdot \mathbf{E}_m$ is the y component of the field distribution of mode m . For a symmetry-protected BIC of TM₁ band, E_{my} with wave vector $\mathbf{k}_{\parallel} = k_y \hat{\mathbf{y}} = \pm 2\pi/p \hat{\mathbf{y}}$ (i.e., considering the Γ point in the second Brillouin zone) can be expressed as $E_{my}(y, \mathbf{R}_0, \omega) = e^{ik_y y} \cdot \mathcal{E}_{my}(\mathbf{R}_0, \omega)$. The master Eq. (4) highlights that the efficient excitation of an eigenmode requires the phase matching $\omega = vk_y$ and the maximum mode-electron overlapping.

Phase matching with the Γ -point BIC mode in TM₁ band (resonance frequency ω_{BIC}) requires the electron velocity v_{BIC} to satisfy the condition $v_{\text{BIC}} = \omega_{\text{BIC}}/(2\pi/p)$. Based on the parameters above, the evaluated velocity is approximated as $v_{\text{BIC}} \approx 0.609c$. In Fig. 2(a), we visualize the phase-matching condition across the TM₁ band. The intersection points (black solid line) between the TM₁ band (Q -factor encoded surface) and the electron dispersion plane (pink transparent plane) are the phase-matched TM₁ modes. The y component of the incident electric field distribution at ω_{BIC} under phase-matching condition is shown in Fig. 2(b), which prominently overlaps with the BIC's mode profile [Fig. 2(d)].

III. EFFECTIVE EXCITATION OF QUASI-BIC AND OPTICAL VORTEX EMISSION

Initial frequency-domain simulations provide an approximate electron beam velocity for phase-matching with an ideal BIC. However, ideal BICs, which are Bloch modes delocalized across an infinite slab, couple poorly with the pointlike electron source. Spatially truncating the PCS would convert the ideal BIC into a quasi-BIC with a finite mode volume

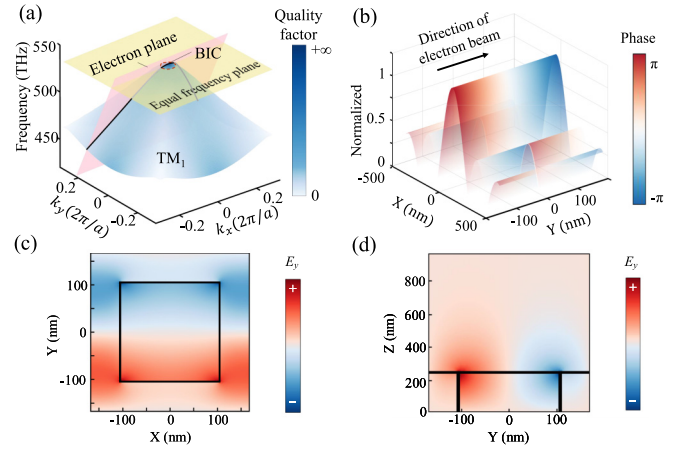


FIG. 2. Efficient coupling between the free electron and the BIC. (a) TM₁ band structure of the PCS with Q factors encoded as color gradients, overlaid with the dispersion plane of the free electron at $v_{\text{BIC}} \approx 0.609c$. The black solid line marks the intersection of the two planes, indicating the phase-matching condition. (b) E_y distribution of the incident field of the free electron (in the frequency domain at $f_{\text{BIC}} = 536.98$ THz) with $v_{\text{BIC}} \approx 0.609c$. E_y distribution of the TM₁ BIC in (c) the XY plane and (d) the YZ plane. The mode profiles are calculated using COMSOL.

and spectral linewidth, while maintaining a high Q factor. To model this, we conduct 3D FDTD simulations on a finite PCS (31×31 unit cells), using the same geometric parameters as those shown in Fig. 1(b). We also conduct simulations of the free electron interaction with a 41×41 unit cell PCS and found that 31×31 unit cells are sufficient to obtain the main results [34]. PMLs are applied to all boundaries, except for the z_{min} boundary where a perfect metal conductor (PMC) condition is used to select the TM mode. The electron beam is modeled as an array of 2500 dipoles spaced 4 nm apart along its trajectory [35,36]. The simulation time is chosen as 2500 fs. We isolate the interaction signal by subtracting the background electric field, which is obtained from an additional simulation without any dielectric structure, from the total calculated field. We normalize the calculated electric field by α and the power by α^2 to obtain the field generated by a single electron [37]. Here, α is a dimensionless quantity given by

$$\alpha = \frac{e \Delta x}{p_{\text{dipole}} s(\omega) \omega},$$

where p_{dipole} is the base amplitude of the dipole source, $s(\omega)$ is the Fourier transform of the source's time signal, and Δx denotes the spacing between adjacent dipoles.

Considering the potential frequency shifts of the quasi-BIC from the ideal BIC condition due to the finite size effect, we need to refine the electron velocity for optimal phase matching. We first analyze the electron's radiative power spectral density as a function of electron energy. As shown in Fig. 3(a), this analysis reveals a pronounced radiation enhancement near the quasi-BIC frequency on the TM₁ band when the electron velocity is $0.604c$. To further verify the coupling, we calculate the electron energy loss probability density at this optimal electron velocity using its definition [first line of Eq. (4)], in

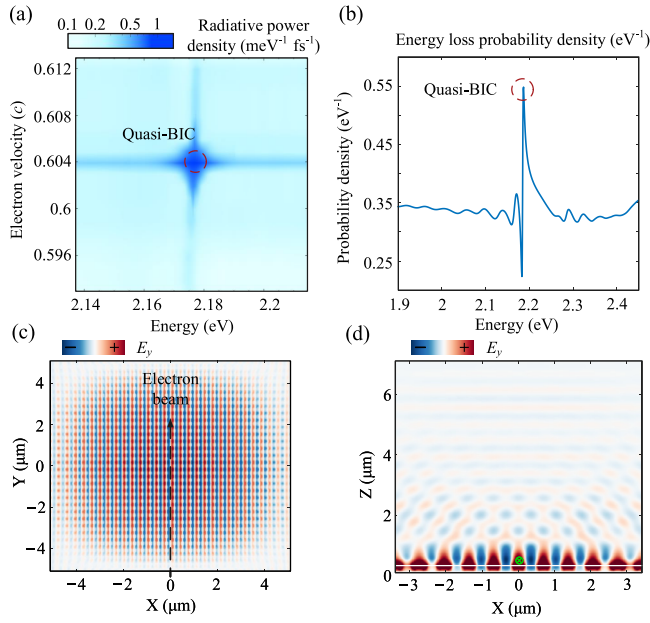


FIG. 3. Effective excitation of a quasi-BIC by a pointlike electron. (a) Radiative power spectral density from a single electron, exhibiting a pronounced peak near the quasi-BIC's single-photon energy. This radiation is significantly enhanced under the phase-matching condition (electron velocity $v_{\text{BIC}} = 0.604c$). (b) Electron energy loss spectral density for a single electron, showing a corresponding peak near the quasi-BIC energy, further confirming efficient mode excitation. (c), (d) E_y field distribution of the mode in (c) the XY plane and (d) XZ plane after the $v_{\text{BIC}} = 0.604c$ electron passes. The distributions closely resemble the field pattern of an ideal BIC, but are confined to a finite number of periods. The white solid line denotes the upper surface of PCS, and the green cross represents the electron beam. These results are acquired by the 3D FDTD method.

which the frequency domain $\mathbf{E}^{\text{ind}}$ is acquired by the Fourier transform of FDTD results. The result shows a distinct peak

near the single-photon energy of the quasi-BIC, which indicates effective coupling between the pointlike electron source and the quasi-BIC mode. Finally, the near-field of PCS after the electron passes, presented for the XY plane [at the upper surface of PCS, Fig. 3(c)] and XZ plane [at $Y = 0$, Fig. 3(d)], clearly resembles the ideal BIC field profiles shown in Figs. 2(c) and 2(d), which further validates the effective excitation of the quasi-BIC. Notably, the radiation from leakage of quasi-BIC is nearly vertical, as shown in Fig. 3(d). The guided resonance mode on TM_1 band follows a parabolic dispersion, which leads to a donut-shaped far-field distribution in k -space. Figure 4(a) shows the far-field intensity and SOP distribution near the Γ point; we also provide the far-field distribution in the whole upper plane in the Supplemental Material [34], from which one can see that near-vertical emission dominates. If we choose a counterclockwise loop as indicated by the orange arrow, the polarization angle $\phi(\mathbf{k})$ will change from 0 to -2π . Therefore, the SOP distribution around the Γ point suggests that the topological charge of the emitted light is -1 , which coincides with that of the BIC. To prove this, we project several oriented circular loops centered around Γ point in k -space onto the normalized Poincaré sphere [38]. Figure 4(b) shows that the loops with the larger radii in k -space are mapped closer to the equator on the Poincaré sphere. The nearly complete coverage of the Poincaré sphere indicates a topological charge of -1 , validating that polarization vector forms a vortex around quasi-BIC.

To introduce the PB phase into the emission and map the polarization singularity onto the phase singularity, we decompose the far-field emission into left-handed circular (LC) and right-handed circular (RC) components. This can be readily achieved using optical elements such as a quarter-wave plate (QWP) and a linear polarizer (LP). The polarization states surrounding quasi-BIC can be represented by

$$\begin{aligned} \mathbf{E}_{\text{far-field}}(\mathbf{k}) &= E_0[\cos(\phi)\hat{\mathbf{e}}_x + \sin(\phi)\hat{\mathbf{e}}_y] \\ &= \frac{E_0}{\sqrt{2}}(e^{-i\phi}\hat{\mathbf{e}}_L + e^{i\phi}\hat{\mathbf{e}}_R). \end{aligned} \quad (5)$$

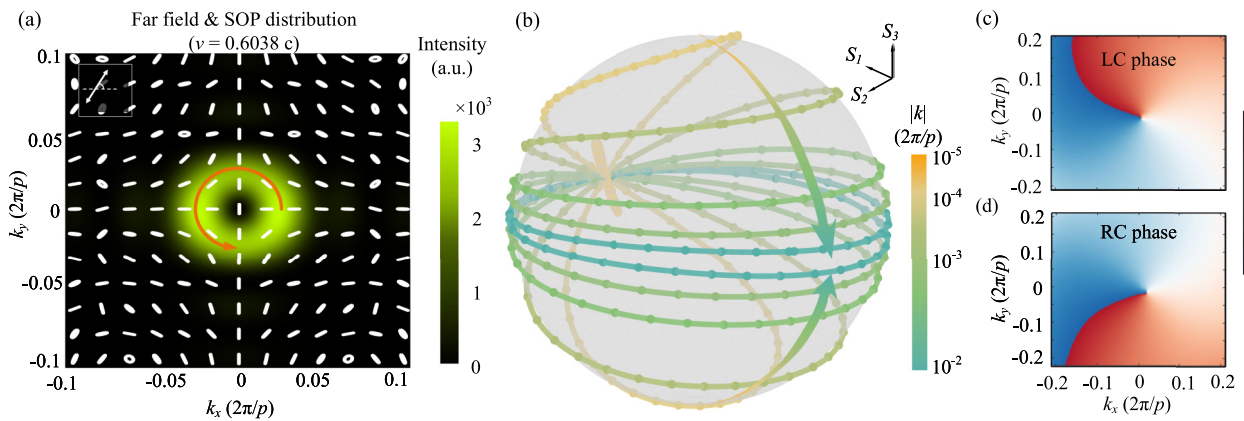


FIG. 4. Intensity, polarization, and phase characteristics of far-field radiation when free electron phase matched with quasi-BIC. (a) Far-field intensity and SOP (represented by polarization ellipse) distribution of the free electron radiation at f_{BIC} . The inset denotes the definition of the polarization angles of SOPs. (b) Circular loops of SOP mapped from the Brillouin zone (a) onto the Poincaré sphere. The loop radii are 6×10^{-5} , 6×10^{-4} , 1×10^{-3} , 3×10^{-3} , and 1×10^{-2} (in units of $2\pi/p$) from orange to green. The coordinates correspond to the three normalized components (S_1 , S_2 , S_3) of the Stokes vector relative to its zeroth component S_0 . Phase distributions of (c) the left-handed and (d) right-handed circular components.

Here, E_0 is the amplitude of the mode, $\phi(|\mathbf{k}|, \varphi)$ is the polarization angle, φ represents the azimuthal coordinate k -space relative to the propagation direction, and $\hat{\mathbf{e}}_L = (\hat{\mathbf{e}}_x + i\hat{\mathbf{e}}_y)/\sqrt{2}$, $\hat{\mathbf{e}}_R = (\hat{\mathbf{e}}_x - i\hat{\mathbf{e}}_y)/\sqrt{2}$ are the LC and RC polarization unit vectors, respectively.

The phase distributions for the LC and RC components are presented in Figs. 4(c) and 4(d). Both components form optical vortex in k -space carrying equal but opposite topological charges (± 1). Within our circular polarization basis convention, the topological charge of the RC component matches that of the polarization vector. This decomposition approach can be generalized to quasi-BICs with arbitrary topological charges, facilitating the generation of electron-beam-driven optical vortex emissions with tailored topological characteristics. Furthermore, the formation of a circular ring structure in k -space [Fig. 4(a)] implies that the corresponding real-space emission manifests as a quasi-Bessel beam, which stems from a superposition of conical wave vectors [24,39]. Both the k -space vortex and the real-space beam exhibit the characteristic azimuthal phase dependence $e^{i\ell\varphi}$, where ℓ denotes the topological charge of the corresponding circular polarization components (in our case, $\ell = +1$ for LC, $\ell = -1$ for RC).

IV. SUMMARY

While this work focused on the interaction with the symmetry-protected BIC at the Γ point of the TM_1 band (which exists as long as symmetry is preserved), the underlying mechanism allows free electrons to interact with other types of BICs as well. As demonstrated in the Supplemental Material [34], free electrons can also efficiently interact with other BIC phenomena, such as merging BICs, which arise from the coalescence of multiple off- Γ BICs with a BIC at the Γ point.

In conclusion, we have demonstrated a novel method for achieving optical vortex radiation through the interaction of free electrons with quasi-BICs on the PCS. Using a uni-

fied framework of free electron-nanophotonic interactions and time domain simulations, we show that the phase-matched electron beams and the maximum mode-electron overlap can efficiently excite BICs, allowing interaction with the truncated photonic structure. The far-field and SOP distributions indicate that coupling between the free electrons and BIC would efficiently result in bright optical vortex emission. We emphasize that the PCS is easy to fabricate and the electron energies employed are readily achievable. Furthermore, the free electrons can also serve as a new tool for probing the dynamic evolution of BIC of PCS, thereby facilitating the control of QED processes and free-electron quantum optics. We envision that the topological charge of free-electron-driven vortex emission can be tailored by achieving phase matching with different bands of PCS or by utilizing structures with higher rotational symmetry. Additionally, the emission angle is adjustable because the position of off- Γ BICs in the k -space can be controlled by modifying the geometric parameters of the PCS. Since the free-electron nearfield can be confined to a spatial region less than 100 nm, it makes free-electron-induced BIC with PCS ideal for the integration of structured nanolasers.

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DATA AVAILABILITY

The data supporting this study's findings are available within the article.

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