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Topological edge states in bichromatic photonic crystals: supplementary material

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This document provides supplementary information to "Topological edge states in bichromatic photonic crystals," https://doi.org/10.1364/OPTICA.6.000096, including details on the computational method, the fitting procedure, and additional spectra of the edge modes for different values of β .

1. GUIDED-MODE EXPANSION METHOD

The full-wave electromagnetic simulations have been computed using a custom implementation of the guided-mode expansion method discussed in Ref. [1]. Here, we provide a brief summary of the computational technique.

The method allows for the solution of the second-order equation for the magnetic field

$$abla imes \left[\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right] = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}).$$
 (S1)

in a three-dimensional system made up of several layers in the z direction. The upper and lower layers are assumed to be homogeneous, whereas the remaining layers include a periodic patterning of the dielectric function in the xy plane, so that the global system is periodic in two dimensions. Calculations of finite-size structures are carried out by assuming a sufficiently large supercell.

For a fixed two-dimensional crystalline momentum **k** in the first Brillouin zone, the magnetic field is expanded over a basis of orthonormal modes:

$$\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = \sum_{\alpha, \mathbf{G}} c_{\alpha, \mathbf{G}} \mathbf{H}_{\alpha, \mathbf{k}+\mathbf{G}}^{(g)}(\mathbf{r}).$$
(S2)

The notation $H_{\alpha,\mathbf{q}}^{(g)}$ indicates the magnetic field of the guided modes of an effective slab waveguide realized by a stack of homogeneous dielectric layers. The dielectric constant of each layer *l* of the effective system is the average of the dielectric constant of the original system in the same layer, i.e., $\overline{\epsilon}_l = (1/A) \int \epsilon_l(x, y) dxdy$, where the integral runs over the two-dimensional unit cell of area *A*. The index α ($\alpha = 1, 2, 3, ...$) refers to the order of the guided mode, whereas **q** is the twodimensional wavevector in the *xy* plane. Upon separating the in-plane and out-of-plane variables, the mode field can be written in the following form:

$$\mathbf{H}_{\alpha,\mathbf{q}}^{(\mathbf{g})}(\mathbf{r}) = e^{i(q_x x + q_y y)} \mathbf{f}_{\alpha,\mathbf{q}}(z), \tag{S3}$$

where $\mathbf{f}_{\alpha,\mathbf{q}}$ is the mode profile function along the *z* axis [2]. Since the effective system is homogeneous in the *xy* plane, in principle the wavevector \mathbf{q} could take any value. However, as the original system is periodic, the nonzero values of \mathbf{q} are restricted to those of the form $\mathbf{q} = \mathbf{k} + \mathbf{G}$, where \mathbf{G} is a two-dimensional reciprocal lattice vector. The mode profile for the guided modes can be derived using the transfer matrix method [2]. The analytical expression of the magnetic field for a three-layer system is also reported in Ref. [1].

Using the expansion in Eq. (S2), the characteristic equation reduces to the linear eigenproblem

$$\sum_{\mathbf{\alpha}',\mathbf{G}'} \mathcal{H}_{(\alpha,\mathbf{G}),(\alpha',\mathbf{G}')} c_{\alpha',\mathbf{G}'} = \frac{\omega^2}{c^2} c_{\alpha,\mathbf{G}}, \tag{S4}$$

with the matrix element

$$\mathcal{H}_{(\alpha,\mathbf{G}),(\alpha',\mathbf{G}')} = \int \frac{1}{\varepsilon(\mathbf{r})} [\nabla \times \mathbf{H}_{\alpha,\mathbf{k}+\mathbf{G}}^{(\mathbf{g})}(\mathbf{r})]^* \cdot [\nabla \times \mathbf{H}_{\alpha',\mathbf{k}+\mathbf{G}'}^{(\mathbf{g})}(\mathbf{r})] d\mathbf{r}.$$
(S5)

In our implementation, we assume a rectangular unit cell of size $L_x \times L_y$, and we truncate the basis of the reciprocal lattice vectors, $\mathbf{G} = (G_x, G_y)$, so that $-2\pi N_x/L_x < G_x \le 2\pi N_x/L_x$ and $-2\pi N_y/L_y < G_y \le 2\pi N_y/L_y$ (N_x and N_y are positive integers). As it can seen with the help of Eq. (S3), the integration over x and y in Eq. (S5) reduces to a Fourier transform, which can be evaluated with the fast Fourier transform algorithm. The remaining integration along z is performed by Gaussian quadrature. Analytical expressions for the integral along z can also be derived [1]. Our truncation scheme differs from the typical



Fig. S1. Dots: fitting results for the parameters of the HAA model in Eq. (S6). The spectrum of each bichromatic structure with varying β has been independently fitted. Red lines: linear regression curves of the fitted parameters.

choice $|\mathbf{G}| < G_{\text{max}}$. The advantage of this truncation is that it removes the ambiguity in the order of carrying out the inversion and the Fourier transform of the dielectric function in Eq. (S5), since the operations of inversion and (discrete) Fourier transform commute for our choice of the reciprocal basis [3].

In all the calculations in this work, we restrict the order of the guided modes to the first (lowest-energy) TE mode. As the system is mirror symmetric with respect to the z = 0 plane, the first TE and TM modes are decoupled by symmetry. We assume a periodic supercell of size $L_y = 8\sqrt{3}a/2$ along the *y* direction. The size along the *x* axis is determined by the geometry of each bichromatic structure, as discussed in the main text. In order to speed up convergence, we employ a simple subpixel isotropic averaging scheme for the dielectric function in the *xy* plane.

2. FITTING PROCEDURE

In order to derive a minimal model to describe the topological behavior of bichromatic structures, we have performed full wave simulations of the spectra of bichromatic structures with $\beta = q/p$, where $q \leq 30$, using the guided-mode expansion method introduced beforehand. The spectra have been computed in the first Brillouin zone for the supercell $[-\pi/(qa) < k \leq \pi/(qa)]$ and for the range of frequencies inside the original photonic crystal (PhC) bandgap. Some illustrative spectra are shown by Fig. 3 in the main text.

Each spectrum for a specific value of β has been independently fitted with the solutions of the generalized Harper-Aubry-André (HAA) model in Eq. (6) of the main text, which we reproduce here in a slightly modified form:

$$\frac{\omega^2}{c^2}c_n = \begin{cases} Vc_n + J_n c_{n+1} + J_{n-1} c_{n-1}, & 1 < n < q, \\ Vc_n + J_n c_{n+1} + J_q e^{-ikqa} c_q, & n = 1, \\ Vc_n + J_1 e^{ikqa} c_1 + J_{n-1} c_{n-1}, & n = q, \end{cases}$$
(S6)

with $J_n = J + J' \cos(2\pi pn/q)$ and n = 1, 2, ..., q. The model describes a periodic chain of particles with position-dependent nearest-neighbor interaction. The fitting parameters are V, J, and J'.

The results of the independent fits are shown in Fig. S1. It was possible to obtain reliable fitting results for approximately $\beta \gtrsim$ 0.75, where there are minibands spanning over the whole PhC bandgap. For $\beta < 0.75$, the frequency extent of the minibands is limited, affecting the amount of information available for the fitting. Moreover, the field profile increasingly deviates from

that of the unperturbed waveguide, reducing the validity of the HAA model in this parameter region. In the range $0.75 \leq \beta \leq 0.96$ we observe that the fitting parameters show a clear linear behavior with β . The dependence of the fitting parameters on β can be justified on physical grounds, since both the energy ground level, V, and the hopping terms, J_n , are affected by the average dielectric function and the hole-hole separation distance in the waveguide, which, in turn, depend on the modified lattice constant a'. Further linear regression analysis of the fitted data led to the linear dependent parameters reported in Eqs. (7) and (8) of the main text (red lines in Fig. S1), which have been used in the HAA results of the main text.

3. EDGE STATES

In the main text, we discuss the formation of edge states for a finite-size bichromatic structure with $\beta = 5/6$. In Fig. S2, we present additional simulations for other values of β . In all cases, we consider finite-sized bichromatic structures encompassing $N_r = 8$ repetitions of the bichormatic supercell embedded inside a larger PhC. We calculate the spectrum as a function of the global spatial displacement of the reduced-size holes, Δ . The full-wave simulations results [Fig. S2(a,c,e,g)] are compared with the solutions of the HAA model for the same values of β [Fig. S2(b,d,f,h)]. The formation of topological edge states crossing the gaps among the minibands of the bichromatic system is evident in all the examples in Fig. S2. The spectral properties of the edge states are analogous to the ones discussed in the main text for the $\beta = 5/6$ case. These results confirm that the existence of the edge states is a general feature of the spectrum of finite-sized bichromatic structures and it is not restricted to a specific value of the parameter β .

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Fig. S2. (a,*c*,*e*,*g*) Full-wave calculations of the frequency eigenvalues of finite-size bichromatic structures as a function of the spatial displacement Δ . In all cases, we assume $N_r = 8$ repetitions of the bichromatic supercell. The value of the parameter $\beta = a' / a$ varies among the examples and it is indicated by the labels. (b,d,f,h) Eigenvalues of the finite-size HAA model in Eqs. (6), (7), and (8) of the main text, for the same values of β .