Supplementary Material for
Point-Defect-Localized Bound States in the Continuum in Photonic Crystals and Structured Fibers

Sachin Vaidya[1], Wladimir A. Benalcazar[1], Alexander Cerjan[1,2,3], Mikael C. Rechtsman[1]

[1]*Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA*
[2]*Sandia National Laboratories, Albuquerque, New Mexico 87123, USA*
[3]*Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque 87123, New Mexico, USA*

Q-FACTOR FOR C_{4v} AND C_{2v} SUPERCELLS

In the main text, we argue that changing the symmetry of the supercell from C_{4v} to C_{2v} allows the defect mode to form a leaky resonance due to a change in the representation of the bulk degeneracy from E to $b_1 \oplus b_2$. This symmetry breaking is achieved by changing the defect site from a circular disc to an elliptical disc with semi-major and semi-minor axes lengths of $0.53a \times t_d$ and $0.4a \times t_d$ respectively where a is the lattice constant and t_d is a tuning parameter. Fig. S1 shows a comparison of quality factors of the defect mode for the two cases and clearly shows the lack of divergence of Q in the C_{2v} symmetric supercell, indicating that the defect mode is indeed a resonance.
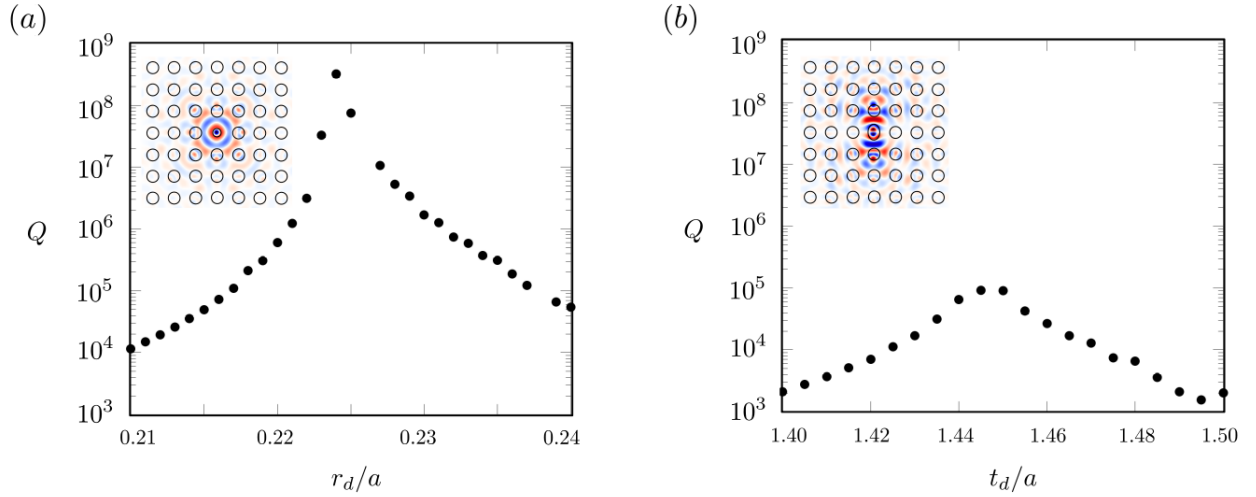

FIG. S1. (a) Quality factor of the defect mode (irrep A_1) in a supercell with C_{4v} symmetry. The divergence in Q shows the appearance of a BIC. (b) Quality factor of a defect mode (irrep b_2) in a supercell with only C_{2v} symmetry. The lack of divergence indicates that the defect mode is a resonance. The insets show the defect mode profiles for parameter values corresponding to the maximum Q.

Q-FACTOR FOR SHIFTED DEFECT SITE

To assess the impact of symmetry breaking due to fabrication imperfections, we consider the same 2D PhC system as discussed in Fig. 2 of the main text. We then calculate the Q-factor of the defect mode from FDTD simulations where the defect site is displaced along the x-direction as shown in Fig. S4 (a). Fig. S4 (b) shows a plot of the Q-factor as a function of the displacement, Δx, normalized to the wavelength of the defect mode, λ_d. As is expected for any symmetry-protected BIC, this perturbation degrades the Q-factor of the BIC. However, we can see that the defect mode still exhibits high Q-factors for typical PhC slab and fiber fabrication errors, which are much less than $\lambda_d/10$. Therefore, any perturbations that are much smaller than the scale of the wavelength will still allow the system to exhibit an ultra-high-Q resonance which includes bends and compressions in the fiber or positional errors in the lattice.
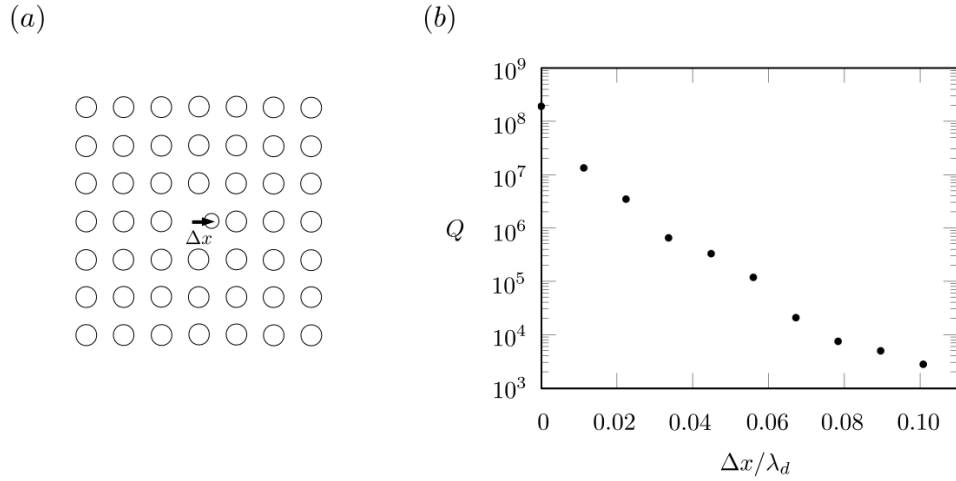
FIG. S2. (a) Displaced defect site inducing a symmetry breaking in the supercell. (b) Quality factor of the defect mode as a function of the normalized displacement of the defect site.

FINDING SPECTRALLY ISOLATED DEGENERACIES IN PHCS USING MPB

The BICs presented in this work can only occur when the bulk band structure exhibits a spectrally-isolated quadratic two-fold degeneracy. Such degeneracies can be found either at Γ or $\mathbf{M}$ in C_{4v} symmetric PhCs or at Γ in C_{3v} and C_{6v} symmetric PhCs. The software package MPB [1] outputs the bandgap along a given trajectory in $\mathbf{k}$-space and provides optimization routines to find bandgaps given some free parameters. Here we describe a method to find isolated degeneracies based on the use of this function. The idea is based on the fact that in a PhC where spectrally-isolated degeneracies occur at HSPs, simply detuning away from HSPs by a small amount $\Delta\mathbf{k}$ results in the opening of a small stop band proportional to $\Delta\mathbf{k}^2$. The structural parameters of the PhC can then be optimized to find these stop bands.

To demonstrate this, we consider the PhC shown in Fig. S2 (a) which consists of three circular discs of radii r_1, r_2 and r_3. The dielectric constant of the high-index material (gray) is $\varepsilon = 2.8$ and that of the low-index material (white) is $\varepsilon = 1$. Using MPB, we run an optimization function on the radii to find the aforementioned stop bands by computing the band structure along the path $(\Gamma + \Delta\mathbf{k_1}) \to \mathbf{X} \to (\mathbf{M} + \Delta\mathbf{k_2}) \to (\Gamma + \Delta\mathbf{k_1})$ for some small $\Delta\mathbf{k_1}$, $\Delta\mathbf{k_2}$. A stop band along the detuned path and hence the required degeneracy is found between TM bands 7 and 8 at Γ for $r_1/a = 0.0924$, $r_2/a = 0.4066$ and $r_3/a = 0.4238$, as shown in Fig. S2 (b).
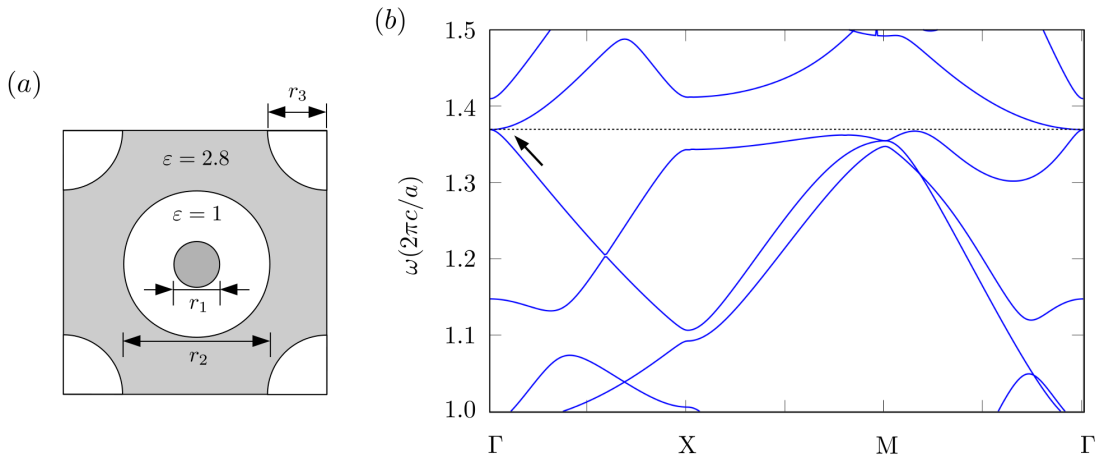

FIG. S3. (a) The PhC design with three parameters: r_1, r_2, and r_3 made out of a dielectric material with $\varepsilon = 2.8$ (b) TM bands of the PhC shown in (a) for optimized values $r_1/a = 0.0924$, $r_2/a = 0.4066$ and $r_3/a = 0.4238$. The spectrally isolated degeneracy occurs at Γ and is marked with an arrow.

SUPERCELL BAND STRUCTURES FOR IDENTIFYING DEFECT MODES

Besides using FDTD, a second way to identify the presence and symmetries of the defect modes is by examining the band structure of a reasonably sized supercell of a PhC with periodic boundaries that contains a defect. To illustrate this, we consider the TM modes of a 2D PhC made of circular discs with $r = 0.15$ and $\varepsilon = 6$. This PhC exhibits the spectrally isolated degeneracy between its second and third TM bands. We introduce a defect in this supercell by detuning the radius of the central disc and plot the band structure of this supercell going through the high symmetry points of its small Brillouin zone. Fig. S3 (a) shows that the bulk degeneracy can still be clearly seen at the new **M** point in the folded band structure. The defect modes are easily identified by characteristic flat bands in the dispersion of this supercell. Moreover, as the defect radius is varied, the frequencies of the bulk states which have support on all sites of the supercell are barely affected but the frequencies of the defect localized modes are strongly affected. We can then see the effect of tuning the defect size in middle panel of Fig. S3 (a) where the symmetry mismatch between the bulk and defect modes allows for a fine-tuned three-fold degeneracy to occur. The absence of any avoided crossings indicates the formation of a BIC due to a lack of mixing between the bulk and defect modes.
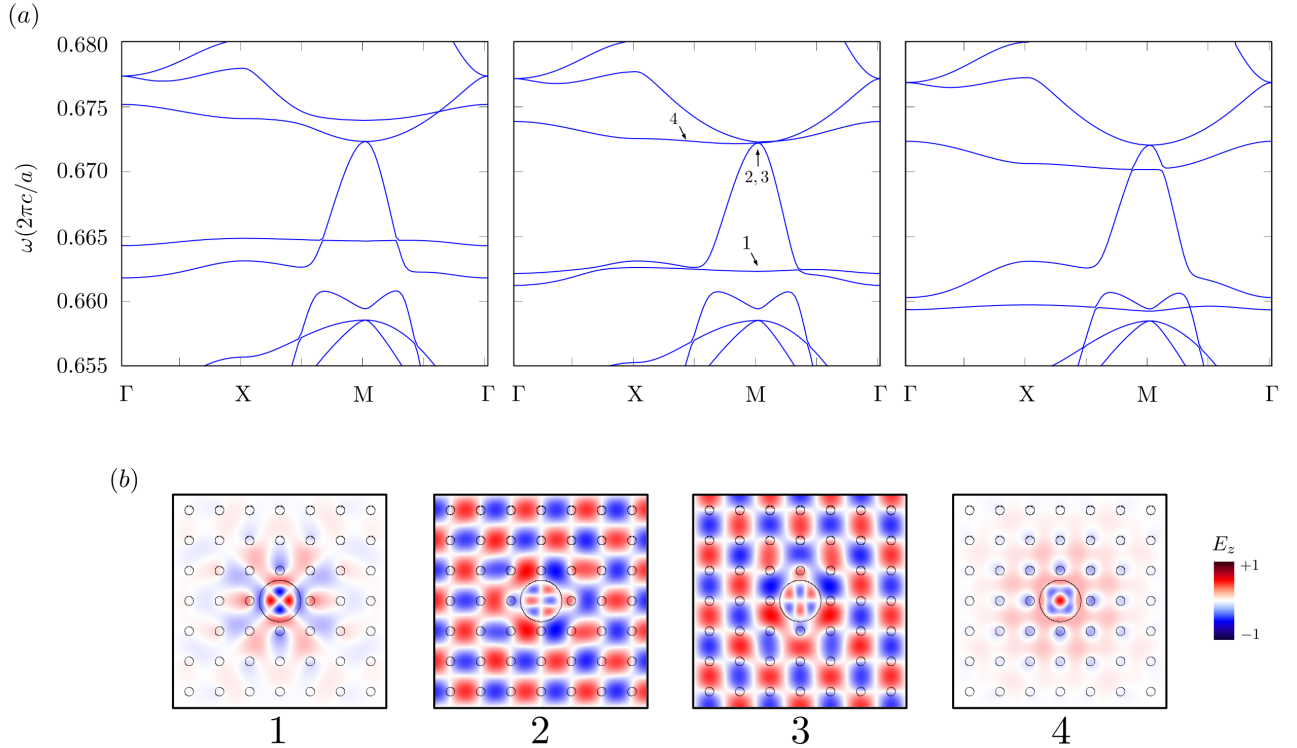
(a)

(b)

FIG. S4. (a) The band structure of a supercell consisting of 7x7 sites with periodic boundary conditions. The defect introduced in the center has radii 0.69a, 0.695a and 0.7a in the three sub-plots (left to right). The middle panel shows that the defect mode can be fine-tuned to be degenerate with the spectrally isolated two-fold degeneracy of the bulk. (b) z-component of **E**-field of the defect modes labelled 1 and 4 (irreps B_1 and A_1 respectively) and the two modes of the bulk degeneracy labelled 2 and 3 (irrep E).

[1] S. G. Johnson and J. D. Joannopoulos, Opt. Express **8**, 173 (2001).