Selection Rules for Symmetry-Protected Bound States in the Continuum

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Photonic crystal slabs (PCSs) are a well-studied class of devices known to support optical Fano resonances for light normally incident to the slab, useful for narrowband filters, modulators, and nonlinear photonic devices. In shallow-etched PCSs the linewidth of the resonances is easily controlled by tuning the etching depth. This design strength comes at the cost of large device footprint due to the poor in-plane localization of optical energy. In fully-etched PCSs realized in high index contrast material systems, the in-plane localization is greatly improved, but the command over linewidth suffers. This disadvantage in fully-etched PCSs, also known as high contrast gratings (HCGs), can be overcome by accessing symmetry-protected Bound States in the Continuum (BICs). By perturbing an HCG, the BIC may be excited from the free space with an inverse squared dependence on the magnitude of the perturbation, while inheriting the excellent in-plane localization of their unperturbed counterparts. Here, we report an exhaustive catalogue of the selection rules (if and to which free space polarization coupling occurs) of BICs controlled by in-plane symmetry breaking in six types of two-dimensional PCS lattices. The chosen lattices allow access to the three highest symmetry mode classes of unperturbed square and hexagonal PCSs. The restriction to in-plane symmetry allows for devices realized with simple lithographic fabrication techniques in comparison to out-of-plane symmetry breaking, useful for practical applications. The approach reported provides a high-level roadmap for designing PCSs supporting tunable sharp spectral features in a mature fabrication platform with minimal device footprint.

I. INTRODUCTION

Enhancement of light-matter interactions is a key capability for improving and expanding the functionality of a wide gamut of photonic devices. Spatially and temporally confining light enables compact planar optical modulators with fast switching speeds [1–4], narrowband bandpass filters [5–9], sensitive biological and refractive index sensors [10–12], efficient optical micro-electrical mechanical devices [13, 14], novel lasers [15–19], and enhanced nonlinear [20–23] and quantum optical phenomena [24, 25]. This is conventionally achieved by the introduction of an optical cavity, which circulates optical energy, affording a photon many passes through a material.

Planar diffractive optics enable uniquely compact optical confinement in lightweight quasi-two-dimensional systems fabricated by mature micro- and nano-fabrication technologies. Traditional plasmonic materials such as Gold enable impressive light-matter interaction in metasurfaces [23, 26–30], but are incompatible with standard complementary metal-oxide semiconductor (CMOS) foundries. Alternative plasmonic materials are an active area of study [31, 32], but without exception introduce significant optical losses that reduce the efficiency of a photonic device. These limitations motivate exploring methods of confining optical energy without metals, restricting the optical materials to common dielectric materials such as Silicon and its oxide.

A classic example of a dielectric diffractive optical element with enhanced light-matter interactions is the low-contrast grating (LCG), or guided mode resonance filter [5–8]. By periodically corrugating a thin slab with subwavelength periodicity, a laterally propagating waveguide mode supported by the slab may couple to normally incident light. The leakage back out of the slab interferes with the direct optical pathways (here, the Fabry-Perot resonance), producing a well-known Fano resonance [33–35]. Related phenomena have been studied for over a century, beginning with Woods anomalies [36–38]. In an LCG, the degree of corrugation can be easily controlled experimentally, and is a design parameter that directly controls the linewidth of the resonant spectral feature. In particular, for small corrugation the Q-factor of the resonance is known to be inversely related to the depth of the corrugation [39]. However, this attractive design feature comes with an inherent drawback: the long optical lifetime comes from the long distance the guided mode travels within the device before coupling back to free space; the device therefore needs to be of a lateral size larger than this characteristic travel distance in order to observe a significant spectral feature. In other words, LCGs are constrained by a tradeoff between spatial confinement (device size) and temporal confinement (Q-factor).

Another well-studied diffractive optical element is the high contrast grating (HCG) [40–42], known to allow compact devices due to large in-plane Bragg reflection laterally confining optical energy. Since the corrugation is deep (and, typically, complete) in HCGs, the ease of control of the Q-factor by the method present in LCGs is lost. HCGs are best-known for their broadband spectral features for this reason. However, HCGs are also known to support sharp spectral features in the form of Fano resonances [42–44]. In particular, for certain combinations of optical materials, geometries, wavelength, an-

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gle, and polarization, the Q-factor may become infinite, a phenomenon known as a “bound state in the continuum” (BIC) [45–48]. Operating near a BIC in the relevant multi-dimensional parameter space allows tuning of a resonance with finite Q-factor born of interference involving the mode responsible for the BIC. Unfortunately, because of the complex and sensitive dependence on many parameters simultaneously, this control is not robust in comparison to the control in an LCG.

However, HCGs can support two classes of BICs: those excluded from coupling to free space due to symmetry constraints (or “symmetry-protected”), and those excluded for reasons unrelated to symmetry (or “accidental” [49]). It has been argued recently [50] that symmetry-protected BICs in HCGs are better suited than accidental BICs for creating compact optical devices with sharp spectral features. It is well-known that by reducing the symmetry [28, 50–62] of an HCG or PCS, symmetry-protected BICs can be accessed at normal incidence, resulting in Fano resonances with Q-factors controlled by the magnitude of the perturbation. This restores a robust design paradigm for controlling the Q-factor of a sharp spectral feature. Additionally, because the BICs are associated with modes in an HCG, the modes are localized in a manner related to the flatness of the band structure. It has also recently been shown [61, 62] that proper perturbation (including breaking vertical symmetry) allows excellent control of the band structure. Therefore, a symmetry-broken HCG inherits the benefits of both LCGs and HCGs relevant to sharp spectral features in finite devices [50].

In particular, a period doubling perturbation (a dimerization of an HCG) allows modes previously bound (under the light line at the edge of the first Brillouin zone (FBZ)) to be brought into the continuum, coupling to a range of angles near normal incidence to a degree controlled solely by the perturbation [50, 53–55, 57, 61–64]. Consequently, a “dimerized high contrast grating” (DHCG [50]) is an excellent candidate platform for planar optical devices with both spatial and temporal confinement of light. Much of the study of DHCGs has focused on simple, one-dimensional devices, enabling control of the mode in one in-plane direction, but not the orthogonal direction. Two-dimensional PCSs in high index contrast systems with periodic perturbations are the natural extension of DHCGs that solve this limitation, and are the subject of this paper. The number of symmetries in a two-dimensional PCS is significantly greater than the simple one-dimensional case; the wealth of modal interactions between free space and two-dimensional PCSs with periodic perturbation therefore requires detailed exploration.

In this paper, we study the optical response due to planar perturbations applied to high-symmetry PCS lattices. In Sec. B 1, we review symmetry-protected BICs and how they spatially and temporally confine light. In Section II B, we review the classification in the language of Group Theory of the three types of high symmetry modes supported by each square and hexagonal PCS (six types of modes in total). Section III A explores six classes of perturbed lattices chosen to target the six high symmetry modes. To determine the impact of these perturbations, Sec. III B derives the symmetry constrained coupling condition specifying which, if any, free space polarization couples upon perturbation. The degenerated space groups compatible with each unperturbed lattice are exhaustively listed, and in Sec. III C the polarization dependence for each mode and each space group is written down by applying Group Theory principles. The result is a catalogue of the selection rules for symmetry-protected BICs describing all the unique ways that the six highest symmetry modes of square and hexagonal photonic crystal lattices may be accessed by in-plane symmetry breaking. Finally, in Sec. IV we discuss notable aspects of the catalogue and sketch several example device applications.

II. BACKGROUND

A. Symmetry-Protected Bound States in the Continuum

Symmetry-protected BICs are commonly studied in monatomic PCSs, where even/odd symmetry conditions may preclude coupling to free space at normal incidence. Breaking the relevant symmetries (e.g., exciting by off-normal incident light, or obliquely etching a PCS) can then allow coupling to free space, appearing in the transmittance, reflectance, and absorbance (in the presence of loss) spectra as a Fano resonance. The BICs in diatomic PCSs (e.g., DHCGs) are subject to the analogous even/odd symmetry conditions, so that once the period doubling has folded the bound modes into the continuum, they may still be left bound in the continuum. If the relevant even/odd symmetry is broken, the perturbation allows coupling to the BIC. Both the monatomic and diatomic approaches fall under the same category of accessing symmetry-protected BICs, but access distinct high symmetry modes (that is, modes with distinct periodicity and field profiles). Therefore, to fully utilize the available perturbations and modes, we study both monatomic and multi-atomic PCSs.

As an example of a design process of a finite-sized DHCG, we explore a BIC in a diatomic lattice artistically depicted in Fig. 1(a). Figure 1(b) and 1(c) define the geometric parameters of the unperturbed and perturbed lattices, respectively. The two “atoms” (here, pillars of Silicon) in the perturbed lattice are identical in height, H, and diameter, D, and sit in a lattice of period √2P, where P is the period of the unperturbed lattice. The perturbation can be quantified by the difference in the gaps between atoms in both cases: the perturbed gap is g2 = g + δ, where g is the unperturbed gap (g = (P − D)/2) and δ is the perturbation. The FBZ of the unperturbed and the perturbed lattices are
FIG. 1. (a) Artistic rendering of a symmetry-protected bound state in the continuum in a periodically perturbed square lattice. (b) Geometry of the unperturbed lattice. (c) Geometry of the perturbed lattice. (d) First Brillouin zone of the unperturbed lattice, with red arrows tracing the path used in the band diagram of (i). (e) First Brillouin zone of the perturbed lattice, showing band folding. (f,g) Out-of-plane magnetic field and in-plane electric field components of the fundamental mode of the perturbed lattice. (h) Dependence of the Q-factor on the perturbation, $\delta = g_2 - g$. (i) Band diagram (with target band highlighted in red) of the folded modes in a finite height PCS with $D = 0.411 \mu m$, $H = 0.295 \mu m$, $P = 0.527 \mu m$. These parameters correspond an operating wavelength of $\lambda = 1.58 \mu m$ with the optimal (minimal) figure of merit $|F|$ as found by the parameter sweep in (j), in which $|F|$ is mapped for varying $D/P$ and $H/P$. (k) Transmittance, $T$, near the fundamental mode of an infinitely periodic device and a finite device ($30 \times 30 \mu m$) with $\delta = 80 \mu m$ excited by a Gaussian beam with $e^{-2}$ waist radius of $w_0 = 7 \mu m$. Both devices show $Q \approx 1,000$ and excellent resonance visibility, indicating that the performance of the device is maintained despite the finite size.
shown in Fig. 1(d) and 1(e) with high symmetry points defined and the primed coordinates representing the perturbed lattice. The effect of the lattice transformation (taking the period in real space from \( P \) to \( \sqrt{2}P \)) is to shrink the extent of the FBZ and rotate it by 45°. The states belonging to sections of the unperturbed FBZ that lie outside of the new, perturbed FBZ are, by Blochs Theorem, equivalent to states within the new FBZ. They are brought into the new FBZ by translation of a reciprocal lattice vector (a process known as Brillouin Zone folding) as depicted graphically in Fig. 1(e) for the shaded area near the \( X \) point. The bound modes that were at the \( X \) point are now at the \( \Gamma \) point (that is, in the continuum) due to the perturbation.

The new modes brought into the continuum may now couple and produce Fano-like sharp spectral features for normally incident light. By construction, the coupling strength is related to the magnitude of the perturbation. It has been shown \[50\] that the coupling strength for small perturbations is of the order of \( \delta \). Since the Q-factor of a sharp resonance is inversely proportional to the square of the coupling strength \[39\], a symmetry-protected BIC has a Q-factor governed by

\[
Q = C/\delta^2
\]

where the constant \( C \) can vary depending on the mode, geometry, materials, and polarization. Figure 1(f) and 1(g) show the mode profiles for the fundamental mode depicted in Fig. 1(a). Figure 1(h) shows full-wave simulations of the Q-factor for the fundamental mode as a function of perturbation strength, agreeing well with Eq. (1) with \( C \approx 6.5P^2 \). Figure 1(i) contains the band diagram for the structure calculated by the planewave expansion method (PWEM) using the supercell method, with high symmetry points defined relative to both the unperturbed and perturbed lattices.

The band structure in Fig. 1(i) can help predict the accuracy of Eq. (1) for finite devices. In an infinite device, a planewave corresponds to a single state (for instance, a mode at the \( \Gamma \) point) and the band curvature is irrelevant. However, a finite device excited by a Gaussian beam will behave as some combination of responses excited by the planewaves composing that Gaussian beam. One simple model for predicting the behavior of a finite device is to perform a weighted sum of the spectra of the constitutive planewaves \[50\]. We model a band by a Taylor expansion about the \( \Gamma \) point, \( \omega_{res}(k) = \omega_0 + bk^2 \), where \( \omega_0 \) is the angular frequency of the mode at \( k = 0 \) and \( b = \left. \frac{\partial^2 \omega_{res}}{\partial k^2} \right|_{k=0} \). A Gaussian beam with a characteristic spread in wavevector of \( \Delta k \) will excite a characteristic spread of frequencies \( \Delta \omega = b\Delta k^2 \). It is natural to expect that if this spread of frequencies is larger than the linewidth of the resonance, \( d\omega \), excited in an infinite device by a planewave, the spectral feature will be washed out, lowering the observed \( Q \) and invalidating Eq. (1). This suggests a constraint \( Q = \frac{\omega_0}{d\omega} \leq \frac{\omega_0}{\Delta \omega} = \frac{\lambda}{\Delta \lambda} \). In other words, there is an upper limit on the Q-factor attainable in a finite device due to the band curvature near the \( \Gamma \) point.

While this simple model does not account for all of the possible finite size effects, the derived constraint suggests that optimizing the band flatness will tend to allow for the most compact devices. In particular, the factor to minimize is \( F = |b|/\omega_0 \), which serves as a figure of merit when designing a device by computing its band structure. Figure 1(j) maps \( F \) as calculated for a variety of diameters and heights (relative to the period) of Silicon pillars sitting on a Silicon Dioxide substrate. While the curvature is different along \( \Gamma - M' \), or the \( k_x \) direction, compared to along \( \Gamma - X' \), or the \( k_y \) direction, this band is limited by its curvature in the \( k_x \) direction; we therefore restrict the calculation of \( F \) to the band along the \( k_x \) direction.

We choose a design with the smallest \( F \) according to Fig. 1(j) and scale its geometrical parameters by a factor \( \lambda/\lambda_{res} \) such that the operating resonance wavelength is \( \lambda = 1.58\mu m \) for a calculated resonance wavelength, \( \lambda_{res} \). Figure 1(k) shows reflectance spectra calculated by full-wave simulations of an infinitely periodic device excited by a planewave of either \( x \) or \( y \) polarization, demonstrating that this coupling only occurs for \( y \) polarization. Figure 1(k) also shows a simulated reflectance spectrum of a device calculated by full-wave simulations of finite size \((30 \mu m \times 30 \mu m)\) excited by a Gaussian beam with a waist radius of \( w_0 = 7 \mu m \). The spectral feature remains intact, confirming that the flat band calculated in Fig. 1(i) allows for compact devices with moderately high \( Q \approx 10^3 \).

Figure 1 overviews the design process of a compact optical device (a two-dimensional DHCG) supporting a sharp spectral feature due to a symmetry-protected BIC. However, this process represented just one high symmetry mode not accessible by monatomic PCSs, and explored the behavior as a result of only one specific perturbation. This behavior was shown to be weakly dependent on incident angle (Fig. 1(i)), but strongly dependent on incident polarization (Fig. 1(k)). The remainder of this paper will provide a theoretical description allowing prediction of the polarization behavior (selection rules) of all high symmetry modes and perturbations.

### B. Classification of High Symmetry Modes

The first step to determining the selection rules of perturbed PCSs is to classify the modes present. Since the selection rules arise from symmetry breaking, a mode classification scheme employing the symmetries of the allowed modes is the natural choice. Although the final devices of interest are three-dimensional in nature (having a finite thickness in the out-of-plane direction, \( z \)), it considerably simplifies the analysis to begin with Maxwell’s equations in two-dimensions. In this case, Maxwell’s six curl equations decouple into two separate sets of three equations, each set defining modes characterized by ei-
ther the out-of-plane magnetic field, $H_z$, (referred to as TE modes) or the out-of-plane electric field, $E_z$ (referred to as TM modes). Each mode is then definable by this single field component. We therefore select, review, and carry out a Group Theory approach detailed in Ref. [65] to classify the modes by in-plane symmetries of the out-of-plane field component.

Since the fields exist in a periodic lattice, they are characterized by planewaves with magnitudes and directions corresponding to high symmetry points of the reciprocal lattice. When the index contrast is low, this characterization is excellent; when the index contrast is large (such as a Silicon and air system), significant deviations in resonance frequencies occur relative to the low index contrast systems, but the symmetries of the possible modes remain unchanged. The modes can therefore be studied with reference to the extended zone scheme.

Figure 2(a) depicts the extended zone scheme for a square lattice, with notable high symmetry points marked. In particular, the $\Gamma$ points, $M$ points, and $X$ points are labeled by an index pertaining to their distance from the origin, $\Gamma^{(0)}$. These points have point group symmetries $C_{4v}$, $C_{2v}$, and $C_{4v}$, respectively (see Appendix A for the character tables and other relevant Group Theory tables), and the modes decomposable by planewaves corresponding to these points are describable by these point groups. These three sets of points are the highest symmetry points in the reciprocal lattice, and therefore

| Group  | Point | N | $k$ | $\frac{2\pi}{a}$ | Irreducible Representations |
|--------|-------|---|-----|------------------|-----------------------------|
| $C_{4v}$ | $\Gamma^{(0)}$ | 1 | 0 | | $A_1$ |
| | $\Gamma^{(1)}$ | 4 | 1 | | $A_1 + B_1 + E$ |
| | $\Gamma^{(2)}$ | 4 | $\sqrt{2}$ | | $A_1 + B_2 + E$ |
| | $\Gamma^{(3)}$ | 4 | 2 | | $A_1 + B_2 + E$ |
| | $\Gamma^{(4)}$ | 8 | $\sqrt{5}$ | | $A_1 + A_2 + B_1 + B_2 + 2E$ |
| $C_{2v}$ | $M^{(1)}$ | 2 | 1/2 | | $A_1 + B_1$ |
| | $M^{(2)}$ | 4 | $\sqrt{5}/4$ | | $A_1 + A_2 + B_1 + B_2$ |
| | $M^{(3)}$ | 2 | 3/2 | | $A_1 + B_1$ |
| | $M^{(4)}$ | 4 | $\sqrt{13}/2$ | | $A_1 + A_2 + B_1 + B_2$ |
| $C_{4v}$ | $X^{(1)}$ | 4 | $\sqrt{17}/2$ | | $A_1 + A_2 + B_1 + B_2 + 2E$ |
| | $X^{(2)}$ | 8 | $\sqrt{5}/2$ | | $A_1 + A_2 + B_1 + B_2 + 2E$ |
| | $X^{(3)}$ | 4 | 2 | | $A_1 + B_2 + E$ |
| | $X^{(4)}$ | 8 | $\sqrt{13}/2$ | | $A_1 + A_2 + B_1 + B_2 + 2E$ |

FIG. 2. Extended zone scheme mode classification. (a,b) Extended zones in reciprocal space of the square and hexagonal lattices. (c,d) Mode classification tables for the square and hexagonal lattices detailing the point group (column labeled “Group”), extended zone (column labeled “Point”), number of modes (column labeled “N”), characteristic magnitude of the planewave (column labeled “$\frac{2\pi}{a}$”), and the irreducible representations (mode symmetries) present at each extended zone for each of the six high symmetry mode types.
### FIG. 3. Modes at the high symmetry points in the square lattice, classified by in-plane symmetries (column-wise) and extended zone (row-wise). The three tables correspond to the modes at the Γ, M, and X points, respectively. Modes are calculated by planewave expansion method for the electric field out of plane; an analogous set exists with magnetic field out of plane.

| $C_{4v}$ | $\Gamma^{(1)}$ | $\Gamma^{(2)}$ | $\Gamma^{(3)}$ | $\Gamma^{(4)}$ | $C_{2v}$ | $M^{(1)}$ | $M^{(2)}$ | $M^{(3)}$ | $M^{(4)}$ | $C_{4v}$ | $X^{(1)}$ | $X^{(2)}$ | $X^{(3)}$ | $X^{(4)}$ |
|----------|----------------|----------------|----------------|----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| $A_1$    |                |                |                |                | $A_1$    |          |          |          |          | $A_1$    |          |          |          |          |
| $A_2$    | -              | -              | -              |                | $A_2$    | -        | -        | -        | -        | $A_2$    | -        | -        | -        | -        |
| $B_1$    | -              |                | -              |                | $B_1$    | -        | -        | -        | -        | $B_1$    | -        | -        | -        | -        |
| $B_2$    | -              | -              |                |                | $B_2$    | -        | -        | -        | -        | $B_2$    | -        | -        | -        | -        |
| $E$      |                |                |                |                |          |          |          |          |          | $E$      |          |          |          |          |

### FIG. 4. Modes at the high symmetry points in the hexagonal lattice, classified by in-plane symmetries (column-wise) and extended zone (row-wise). The three tables correspond to the modes at the Γ, M, and K points, respectively. Modes are calculated by planewave expansion method for the electric field out of plane; an analogous set exists with magnetic field out of plane.

| $C_{6v}$ | $\Gamma^{(1)}$ | $\Gamma^{(2)}$ | $\Gamma^{(3)}$ | $\Gamma^{(4)}$ | $C_{2v}$ | $M^{(1)}$ | $M^{(2)}$ | $M^{(3)}$ | $M^{(4)}$ | $C_{6v}$ | $K^{(1)}$ | $K^{(2)}$ | $K^{(3)}$ | $K^{(4)}$ |
|----------|----------------|----------------|----------------|----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| $A_1$    |                |                |                |                | $A_1$    |          |          |          |          | $A_1$    |          |          |          |          |
| $A_2$    | -              | -              | -              |                | $A_2$    | -        | -        | -        | -        | $A_2$    | -        | -        | -        | -        |
| $B_1$    | -              |                | -              |                | $B_1$    | -        | -        | -        | -        | $B_1$    | -        | -        | -        | -        |
| $B_2$    |                | -              |                |                | $B_2$    | -        | -        | -        | -        | $B_2$    | -        | -        | -        | -        |
| $E_1$    |                |                |                |                |          |          |          |          |          | $E_1$    |          |          |          |          |
| $E_2$    |                |                |                |                |          |          |          |          |          | $E_2$    |          |          |          |          |
correspond to the modes of interest in the square lattice. The three analogous sets of points in the hexagonal lattice (Fig. 2(b)) are the Γ points, M points, and K points.

A Group Theory approach \[65-67\] predicts the number and nature of the modes from each set of high symmetry points in the extended zone scheme. Figure 2(c) contains a table summarizing the modes possible at each of the high symmetry points in the square lattice. The degeneracy of a set of high symmetry points, \(N\), is also the number of modes corresponding to that set. The magnitude of the wavevectors, \(k\), of the planewaves of a mode will correspond to the expected eigenfrequencies of the modes (however, as noted above, this correspondence is poor in high index contrast systems). Lastly, the irreducible representations describe the mode symmetries. That is, modes that “transform like” (share all the symmetries of) each irreducible representation listed in an extended zone will be present at that extended zone. Note that the \(E\) irreducible representations are doubly degenerate, and so account for two modes.

Figures 3 and 4 depict the TM modes from the first four extended zones of each high symmetry point in the square and hexagonal lattices, respectively. An analogous set exists for TE modes, identical in symmetries (in \(H_2\) instead of \(E_z\)) but spatially distorted and differing in eigenfrequency. The modes are organized by the extended zone order (columns) and irreducible representation (rows). Reference to the relevant character tables (Appendix A, Fig. A 1(a)) shows that modes labeled by a given irreducible representation transform the same way as the corresponding row in the character table: a 1 in a column of this row means the mode will be symmetric under the class of operations of that column; a \(-1\) means anti-symmetric; a 0 means not symmetric; and a magnitude of 2 signifies that the mode is degenerate.

Finally, the out-of-plane property of the modes is characterized by the order, or of number of anti-nodes, per atom of the PCS in the \(z\) direction. The inclusion of out-of-plane characteristics captures all the relevant features of the modes within the scope of this paper if the PCS has mirror symmetry about an \(xy\) plane. However, if this symmetry is broken (for instance, by the presence of a substrate), then the simplification used here to analyze the modes in two dimensions is not strictly valid. For instance, two-dimensional PCS with a substrate are known to exhibit chiral behavior: incident circularly polarized light can behave in a manner depending on the handedness \[63, 68\]. This behavior of circularly polarized light is omitted here; for linear polarization, the present description suffices even with a substrate.

With the in-plane and out-of-plane features of each mode classified, we are motivated to provide a naming scheme. We call a mode:

\[
\psi_L^{m,n}_{S},
\]

where \(\psi\) is TM or TE if the mode is characterized by \(E_z\) or \(H_2\) respectively, \(L\) signifies the reciprocal lattice point (e.g., \(\Gamma\)), \(S\) is the irreducible representation (e.g., \(A_1\)), \(m\) is the extended zone order, and \(n\) is the out-of-plane order. For instance, the mode in the \(B_2\) row and \(X^{(1)}\) column in Fig. 3, with a single out-of-plane anti-node per unit cell of the PCS would be called \(TM_{X,B_2}^{1,1}\), which is the lowest frequency \(E_z\) mode in this square lattice. \(TE_{X,B_2}^{1,1}\) is the mode explored in Fig. 1.

Finally, we note that the \(K\) point modes for the hexagonal lattice are more complex than the other five high symmetry modes. In particular, the \(K\) point in the unperturbed lattice has site symmetry of \(C_{3v}\), as evident in Fig. 2(b). However, there are two identical sets of these \(K\) points; the set not pictured in Fig. 2(b) can be obtained by reflection about the \(k_y\) axis. As demonstrated in Fig. 1, the modes only become BICs once folded to the \(\Gamma\) point by an appropriate perturbation (depicted in Fig. 5). For \(K\) point modes, the analogous perturbation results in a triatomic lattice and therefore triple the number of modes at the new \(\Gamma\) point compared to the unperturbed monatomic lattice. At the perturbed \(\Gamma\) point, a set of modes originating from each set of \(K\) points will mix in pairs. The symmetries of the mixed modes are described by the direct product group \(C_x \otimes C_{3v}\), corresponding to the relationship of the two sets of \(K\) points. This direct product group is isomorphic to (shares the same character table as) the group \(C_{6v}\), allowing the modes to be named in \(C_{6v}\). Naming the modes according to \(C_{6v}\) is inconsistent with the modes in an unperturbed lattice at a single \(K\) point, but consistent with the modes upon folding to the \(\Gamma\) point and mixing in the relevant perturbed lattice. Since our goal is to study these modes in the perturbed lattice, defining the modes in \(C_{6v}\) is the more fruitful choice.

### III. SELECTION RULES

By proper periodic perturbation, any of the six classes of high symmetry modes can be accessed from free space if additional symmetry constraints are satisfied. These symmetry constraints can be treated with a Group Theory approach, and result in a catalogue detailing how each high symmetry mode classified above couples to free space under a given planar perturbation. In the following, we identify six lattice types chosen to target the six high symmetry modes (Fig. 5), list all the degenerated space groups compatible with those lattice types (Fig. 6), and then derive the selection rules for every case (exemplified in Figs. 7 and 8). The resulting catalogues (Figs. 9 and 10) can be used as a high-level roadmap in the design of planar photonic devices.

#### A. Target Space Groups

The six types of high symmetry modes described above motivate six types of lattices, each one uniquely targeting one of the six high symmetry mode types. For each of these lattices, an exhaustive list of lattices with lower
The symmetry degeneration from higher symmetry to lower symmetry will constrain which polarization, if any, may couple to free space for each high symmetry mode. The six lattice types, depicted in Fig. 5, are named based on the modes they target and whether they begin with square or hexagonal symmetries. For instance, the \( Sq \) is a monatomic photonic crystal with a square lattice where the perturbation has periodicity equal to that of the unperturbed lattice. This lattice is labeled by \( \Gamma \) because it supports none of the other types of mode of interest supported by the square lattice (that is, \( M \) and \( X \) modes) in the continuum. Figure 5 (top left) depicts an example real space lattice, First Brillouin Zone (FBZ), and band diagram for \( Sq \) lattice. The white region in the band diagram is the region of the continuum of interest, wherein only the 0th diffractive order is allowed. We constrain ourselves to the area near the \( \Gamma \) point of the white region, where the symmetry-protected BICs can produce sharp spectral features described above.

The \( Sq_M \) lattice (top middle of Fig. 5), on the other hand, is a photonic crystal with perturbations with periodicity double that of the unperturbed lattice in a single direction. This period doubling (in the \( x \) direction in Fig. 5) halves the extent of the FBZ in the \( k_x \) direction. The shaded portion outside the new FBZ is then translated into the FBZ by a reciprocal lattice vector. As a result, the \( M \) point of the unperturbed lattice overlaps with the \( \Gamma \) point, bringing the \( M \) points into the continuum in an analogous way described in the example in Fig. 1. This Brillouin Zone folding also changes the shape of the 0th order diffraction region of the band diagram. The \( \Gamma \) point will now have both the modes at the unperturbed \( \Gamma \) point as well as the \( M \) points. The \( Sq_M \) lattice is the only lattice in Fig. 5 to bring the \( M \) point modes of a square lattice into the continuum, motivating
its name. The remaining lattices target $X$ modes of the square lattice ($S_qX$, which is the lattice type explored in Fig. 1), and $\Gamma$, $M$, and $K$ point modes of the hexagonal lattice ($H_{ex}, H_{exM},$ and $H_{exK}$, respectively) in an analogous way. Notably, two distinct regions are folded in the FBZ of the $H_{exK}$ lattice: as discussed above, two sets of modes are folded to the $\Gamma$ point, one from each distinct $K$ point.

We note that the six lattices chosen in Fig 5 are not an exhaustive set: lattices with any number of atoms per unit cell are possible. Ordering this list of lattices by number of atoms per unit cell, the six chosen lattices are the lowest order lattices uniquely targeting the six high symmetry modes of interest. Appendix B describes three examples of higher order lattices. The approach described in what follows may be used to generate the catalogue for any higher order lattice.

Next, the space groups of degenerated lattices that are compatible (attainable through perturbation) with each lattice are determined and reported in Fig. 6, the space group compatibility table. First, all 17 “wallpaper groups” are listed and categorized by the compatible lattice family (e.g., “Rectangular”). The point group of each of these is given for reference. Then, for each target lattice type (e.g., $S_qX$) the space groups compatible with the lattice class (that is square or hexagonal) are listed. For instance, the space group $p6mm$ requires hexagonal tiling, and is therefore omitted as a possibility for any $S_q$ lattice. Likewise, a $H_{ex}$ lattice cannot be perturbed into a square lattice without distortion of the lattice vectors, but it can be perturbed into a rectangular lattice. The space groups of the square lattice family are therefore omitted from all $H_{ex}$ lattices, but those of the rectangular lattice family are not.

Next, the glide reflection operation (a reflection and a translation by a fraction of a unit cell) is tested for each type of lattice. Glide reflections are present in only some two-dimensional space groups and are not compatible with all of the six target lattice types. As an example, it is quickly found by inspection that $S_q$ do not support glide symmetries in directions other than along the diagonals (more rigorously, in the language of crystallography, monatomic PCSs are incompatible with non-symmetric space groups). This excludes the space groups $pg$, $pgg$, and $pgm$, which are correspondingly greyed out in the column for $S_q$. For the same reason, for the $S_qM$ lattice, glide planes along the direction where the lattice is unperturbed (and therefore monatomic) are incompatible (the $y$ direction in Fig. 5). Additionally, all diagonal glides are incompatible for the $S_qM$ lattice because they correspond to reflection axes that are not included in the point group of any $S_qM$ lattice. This excludes $cm$, $pg$, and $cmm$ for $S_qM$, which are greyed out accordingly. There are no such constraints for the $S_qX$ lattice, which can be degenerated into a lattice of any space group (except the hexagonal ones). Similar arguments can be made for the $H_{ex}$ lattices, and the results are reported in Fig. 6.

Finally, it must be noted that there exist multiple high symmetry points in each real space lattice. These are given names in Fig. 5 for each case. For instance, the $S_q$ lattice has two points having the full symmetry of the $C_4v$ point group, named $\gamma$ and $\xi$. Both are perfectly acceptable to choose as the reference point: in the mode naming scheme in Sec. II B, the $\xi$ point is the reference point, but the modes may all be renamed according to the $\gamma$ point if desired. Similarly, a degenerated space group may choose either of these points to have in common with the unperturbed lattice. Generally speaking, every degenerated space group may be tried with each of the high symmetry points in common with the unperturbed lattice, thereby allowing for more than a single unique example of each space group in each lattice. For instance, there are three distinct $cmm$ space groups in the $S_qX$ catalogue (see Fig. 9): one with the $\gamma$ point as the high symmetry point in common, one with $\xi$, and the last with $\mu$ (which is the space group of the perturbation in Fig. 1). As shown in Fig. 9, though these have identical space groups, they do not have identical selection rules because they are attained through distinct perturbations. Therefore, to determine all of the unique symmetry degenerations possible, an attempt is made to construct each compatible space group (Fig. 6) with

| Lattice | Point group | Space group | $Sq\Gamma$ | $SqM$ | $SqX$ | $Hex\Gamma$ | $HexM$ | $HexK$ |
|---------|-------------|-------------|------------|--------|--------|-------------|--------|--------|
| Oblique | $C_1$       | $p1$        | $p1$       | $p1$   | $p1$   | $p1$        | $p1$   | $p1$   |
|         | $C_2$       | $p2$        | $p2$       | $p2$   | $p2$   | $p2$        | $p2$   | $p2$   |
|         | $C_3$       | $p3$        | $p3$       | $p3$   | $p3$   | $p3$        | $p3$   | $p3$   |
|         | $C_{2v}$    | $p4$        | $p4$       | $p4$   | $p4$   | $p4$        | $p4$   | $p4$   |
|         | $C_{4v}$    | $p4m$       | $p4m$      | $p4m$  | $p4m$  | $p4m$       | $p4m$  | $p4m$  |
|         | $C_3$       | $p6$        | $p6$       | $p6$   | $p6$   | $p6$        | $p6$   | $p6$   |
|         | $C_{4v}$    | $p6mm$      | $p6mm$     | $p6mm$ | $p6mm$ | $p6mm$      | $p6mm$ | $p6mm$ |

**FIG. 6.** Space group compatibility table. Different lattice families (column 1) are compatible with various point groups (column 2), each of which can be further subdivided into the 17 “wallpaper groups” (or two-dimensional space groups, column 3). The remaining columns track the compatible space groups of each degenerated lattice studied. A blank entry means that corresponding space group is excluded due to a mismatch in lattice family; a greyed entry means it is excluded because it has an incompatible glide symmetry.
each high symmetry point in common between the unperturbed and perturbed lattice. The successful attempts comprise the set of all degenerated lattices compatible with those chosen in Fig. 5. This proof by exhaustion is omitted here. For each of these degenerated lattices, the modes derived in the previous section can be studied, and their selection rules derived. The results are tabulated in Figs. 9 and 10 following the methods derived in Secs. III B and III C.

**B. Deriving the Coupling Condition**

To derive the selection rules reported in Figs. 9 and 10, we begin by determining the coupling from free space to vertically propagating waveguide modes with symmetries classified in Section II B. In particular, we determine unvertically propagating waveguide modes with symmetries we begin by determining the coupling from free space to incident field to be a normally incident planewave, with electric field

\[
\mathbf{E}_{\text{inc}}^* = \begin{bmatrix} A_x \\ A_y \\ 0 \end{bmatrix},
\]

and magnetic field

\[
\mathbf{H}_{\text{inc}}^* = \frac{1}{\eta_0} \begin{bmatrix} A_y \\ A_x \\ 0 \end{bmatrix},
\]

where \(\eta_0\) is the impedance of free space. And the mode has electric field

\[
\mathbf{E}_{\text{mode}} = e^{i(\beta z - \omega t)} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix},
\]

and magnetic field

\[
\mathbf{H}_{\text{mode}} = e^{i(\beta z - \omega t)} \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix},
\]

where \(\beta\) is the propagation constant satisfying the dispersion relation \(\omega = c\beta\). Evaluating the cross-products in Eq. (3), the free-space coupling coefficient is written as

\[
\gamma_e \propto \int_A \left[ A_x (\eta_0 H_y + E_x) + A_y (\eta_0 H_x + E_y) \right] dx dy. \tag{4}
\]

Using Maxwells curl equations, the in-plane components \((E_x, E_y, H_x, H_y)\) are replaced with the out-of-plane components \((E_z, H_z)\) to both simplify the equation and allow the previous mode classification scheme (based on the out-of-plane field components) to straightforwardly apply. The resulting form is

\[
\gamma_e \propto \int_A \left[ A_x [c_1 \partial_x E_z + c_2 \partial_y H_z] + A_y [c_1 \partial_y E_z + c_2 \partial_x H_z] \right] dx dy \tag{5}
\]

where

\[
c_1 = \frac{1}{i\beta} \frac{1 + \varepsilon_r(x, y)}{1 - \varepsilon_r(x, y)} \tag{6}
\]

and

\[
c_2 = \frac{2\eta_0}{i\beta} \frac{1}{1 - \varepsilon_r(x, y)} \tag{7}
\]

with the replacement \(\varepsilon_r(x, y) = \varepsilon(x, y)/\varepsilon_0\) as the relative permittivity. This can be written more compactly as

\[
\gamma_e \propto \left\langle [A_x, A_y] \cdot \begin{bmatrix} c_1 \partial_x & c_2 \partial_y \\ c_1 \partial_y & c_2 \partial_x \end{bmatrix} \cdot \begin{bmatrix} E_z \\ H_z \end{bmatrix} \right\rangle \tag{8}
\]

where angled brackets indicate integration over a unit cell. While it is possible to proceed with this form by considering the symmetries of each component, it is considerably simpler and more informative to reduce this to individual choices of incident polarization (e.g., choose \(A_x = 0\) and mode type (i.e., choose either TM modes or TE modes). In this case, we write

\[
\gamma_e \propto \int_A c_j \partial_j \psi dx dy \tag{9}
\]

where \(\psi\) is TM or TE, \(\partial_j\) refers to the partial derivative in a relevant high-symmetry direction \((i = x, y, a, b)\), and \(c_j\) is \(c_1\) when \(\psi\) is TM and \(c_2\) when \(\psi\) is TE.

**C. Determining the Selection Rules**

We now apply Eq. (9) to the modes supported by a PCS. The modes in the unperturbed lattice can be described as the eigenvectors of an eigenvalue equation

\[
H^0 \psi^0 = \mathcal{E}^0 \psi^0 \tag{10}
\]

where the superscript marks reference to the unperturbed eigenvalue problem. We are interested in particular in the \(\psi^0\) that are uncoupled to free space (i.e., \(\psi^0\) for which the integral in Eq. (9) vanishes) due to symmetry. To proceed we apply perturbation theory to determine any non-vanishing terms present in the generalized eigenvalue problem of a degenerated lattice:

\[
H \psi = \mathcal{E} \psi \tag{11}
\]
where $H = H^0 + V$ is perturbed by the perturbation operator, $V$, and $\psi = \psi^0 + \psi^1$ is the perturbed field profile with $\psi^1$ as the first order correction. First order perturbation theory gives the form of the $n^{th}$ mode $\psi_n^1$ as

$$
\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 V \psi_n^0 \rangle}{E_m - E_n} \psi_m^0.
$$

(12)

That is, the perturbed portion of the field is a superposition of the unperturbed fields. (Note that Eq. (12) is the non-degenerate form of perturbation theory, but it can be applied to degenerate states as well if the “correct” orthogonal linear combination of states is known ahead of time. Since these will correspond to a high symmetry direction of the unperturbed fields, they are easy to predict; we therefore use this form to apply to degenerate modes.)

However, inspection of the coefficient, $\langle \psi_m^0 V \psi_n^0 \rangle$, in front of each $\psi_m^0$ reveals that not all $\psi_m^0$ will contribute. In particular, there are constraints on the factors $\psi_m^0$, $V$, and $\psi_n^0$: (1) the contributing $\psi_m^0$ must have the same period as the product $V \psi_n^0$, and (2) the integrand as a whole must not have odd symmetry in any in-plane direction.

The process of determining $\psi_0^0$ that satisfy these symmetry constraints can be clarified and expedited in the language of Group Theory. Specifically, if we can determine the irreducible representations of each factor within the integrand, we can find the symmetries of the total integrand by computing the direct product of those irreducible representations. A direct product is an abstract way to obtain the symmetries of the product of two functions $f$ and $g$: if $h = fg$, the symmetries of $h$ may be obtained by performing the direct product of the representations of $f$ and $g$. That is, $\Gamma_h = \Gamma_f \otimes \Gamma_g$, where $\Gamma_h$ is the representation of $h$ in some point group. Since the fields have been classified already in terms of their irreducible representations, we write the irreducible representation of $\psi_{m,n}^0$, as $\Gamma_{m,n}$, and simplify refer to Figs. 3 or 4. Then, we must determine the irreducible representation of $V$, or $\Gamma_V$, which can be achieved following a process described below. We finally write the direct product as $\Gamma_{\text{integrand}} = \Gamma_m \otimes \Gamma_V \otimes \Gamma_n$.

A necessary condition (equivalent to constraint (2) above) for this integral to be non-vanishing is that this direct product must contain a component that transforms as a constant: the oscillatory components do not contribute upon integration over a unit cell. Since a constant is fully symmetric (that is, it transforms as $\Gamma_1$, which is the highest symmetry irreducible representation in every point group), this condition is identical to saying that $\Gamma_{\text{integrand}}$ must contain $\Gamma_1$. Note that this condition is necessary, but not sufficient. For instance, a cosine transforms as $\Gamma_1$ about the origin, but integrates to zero over a period. We can therefore say that $\langle \psi_m^0 V \psi_n^0 \rangle$ is non-vanishing only if $\Gamma_m \otimes \Gamma_V \otimes \Gamma_n = \Gamma_1 + \ldots$

A direct product is easily calculated by referring to the direct product table of the relevant point group (see Appendix A, Fig. A 2). A notable feature of these tables is that two irreducible representations $\Gamma_i$ and $\Gamma_j$ satisfying $\Gamma_i \otimes \Gamma_j = \Gamma_1 + \ldots$ also satisfy $\Gamma_i = \Gamma_j$. Consequently, we can reframe the condition on the integrand, $\Gamma_m \otimes \Gamma_V \otimes \Gamma_n = \Gamma_1 + \ldots$ to be $\Gamma_m = \Gamma_V \otimes \Gamma_n$. In other words, a field $\psi_0^0$ contributes to the perturbed field $\psi_n^1$ only if $\Gamma_m = \Gamma_V \otimes \Gamma_n$. Since $\psi_n^1$ will transform as the components comprising it (that is, the $\psi_m^0$ with non-vanishing integrals), we finally arrive at the conclusion that $\Gamma_{\psi_1} = \Gamma_V \otimes \Gamma_n$. Since the index $n$ refers to any particular mode of interest, we may drop it:

$$
\Gamma_{\psi^1} = \Gamma_V \otimes \Gamma_{\psi^0}.
$$

(13)

In words, the first order perturbed field profile transforms as the direct product of the irreducible representations of the perturbation operator and the unperturbed field profile in question.

Understanding the symmetries of the perturbed portion of the wavefunction allows us to simplify the free-space coupling condition, Eq. (9):

$$
\gamma_c \propto \int_A \int c_j \partial_i \psi \, dx \, dy = \int_A \int c_j \partial_i (\psi^0 + \psi^1) \, dx \, dy
$$

(14)

Since $c_j$ is a function of in-plane permittivity distribution of a perturbed lattice, it is natural to expect that it has a portion that transforms like $H^0$, which we call $c_{H^0}$, and a portion that transforms like $V$, which we call $c_V$. We can write these portions explicitly to first order using the binomial approximation. Taking $c_2 = c_{H^0} + c_V$, for instance, the unperturbed portion is written

$$
c_{H^0} = \frac{2\varepsilon_0}{\eta^2} \frac{1}{1 - \varepsilon_0^2} \varepsilon_0 H^0,
$$

(15)

and the perturbed portion is written

$$
c_V = \frac{\delta \varepsilon_r(x,y)}{1 - \varepsilon_0^2} c_{H^0},
$$

(16)

where $\varepsilon_r(x,y) = \varepsilon_0^2(x,y) + \delta \varepsilon_r(x,y)$ is decomposed into the unperturbed portion, $\varepsilon_0^2(x,y)$, and perturbed portion, $\delta \varepsilon_r(x,y)$, of the relative permittivity. Since $\varepsilon_0^2(x,y)$ transforms as $\Gamma_1$ by construction of the unperturbed lattices, it is evident that $c_{H^0}$ transforms as $\Gamma_1$: for an even function $f(x)$, the function $1/(1 - f(x))$ is also even. Decomposing the factors in $c_V$, it is clear that it transforms as $\Gamma_V$ because $\delta \varepsilon_r(x,y)$ transforms as $\Gamma_V$ by definition of the perturbation, and the remaining factors in $c_V$ transform as $\Gamma_1$ (which acts as the identity in direct products). A similar argument reveals the equivalent result for $c_1$.

We therefore write $\gamma_c$ as the sum of four terms:

$$
\gamma_c \propto \int_A \int c_{H^0} \partial_i \psi^0 \, dx \, dy + \int_A \int c_{H^0} \partial_i \psi^1 \, dx \, dy + \int c_V \partial_i \psi^0 \, dx \, dy + \int A \int c_V \partial_i \psi^1 \, dx \, dy.
$$

(17)

The first term vanishes for symmetry-protected BICs. As described above, $\Gamma_{H^0} = \Gamma_1$, and so, using Eq. (13),
FIG. 7. Graphical derivation of the selection rules for the X point modes in the S\textsubscript{QX} lattice belonging to the \textit{cmcm} space group. The modes are shown in their unperturbed form as calculated by the plane-wave expansion method. Then, they are schematically drawn as perturbed by the perturbation and decomposed into the unperturbed portion and perturbed portion. The green arrows represent the gradient and predict coupling to a free space plane-wave excitation if a net dipole moment is present. The black arrows represent the corresponding free space polarization each mode couples to.

the second terms integrand transforms as $\Gamma_1 \otimes \Gamma_{\delta_1} \otimes \Gamma_V \otimes \Gamma_{\psi^0} \Rightarrow \Gamma_{\delta_1} \otimes \Gamma_V \otimes \Gamma_{\psi^0}$. The third terms integrand straightforwardly transforms as $\Gamma_V \otimes \Gamma_{\delta_1} \otimes \Gamma_{\psi^0}$, identical to the second term (inspection of Appendix A, Fig. A 2 shows that the direct products in question commute). The fourth term vanishes to first-order, because it is the product of two factors of the perturbation. We are therefore left with two non-vanishing terms whose integrands transform identically.

As before, $\gamma_c$ is non-vanishing only if the integrand has a component that transforms like $\Gamma_1$. We therefore arrive at the symmetry constrained coupling condition:

$$\Gamma_{\delta_1} = \Gamma_V \otimes \Gamma_{\psi^0}.$$  \hspace{1cm} (18)

Since a partial derivative in the $i$ direction transforms like a vector in that direction, it also transforms the same as a free space polarization $i$. The physical interpretation of the coupling condition, Eq. (18), then, is that the symmetries of the perturbed part of the field (i.e., $\Gamma_V \otimes \Gamma_{\psi^0}$) must match the symmetries of a free space polarization (i.e., $\Gamma_{\delta_1}$). That is to say, the perturbed field must have a net dipole moment to couple to free space.

The coupling condition is equivalent to considering whether the integral

$$\gamma_V \propto \int \int_A \partial_i (V \psi^0) \, dx \, dy$$  \hspace{1cm} (19)

vanishes. This form justifies a convenient and insightful graphical method \cite{58} of determining whether $\gamma_c$ is non-zero, without directly determining $\psi^i$, which is not obvious at first glance at Eq. (12). The perturbed mode can be simply drawn by altering the magnitude of the unperturbed field according to the shape and sign of the perturbation. Then, this new perturbed field is decomposed into the unperturbed portion and the perturbed portion (corresponding to $V \psi^0$). Taking the derivative amounts to treating the product $V \psi^0$ as "charges" and the gradient as the "moment"; then, if there is a net dipole moment, the mode couples to the corresponding
free space polarization. Figure 7 depicts this process for determining the selection rules of the TM$^{m,n}$ modes in a $cmm$ lattice with a $cmm$ space group (the same used in Fig. 1). The polarization depicted corresponds to the out-of-plane field component. That is, if $\psi^0$ is a TE (TM) mode, the polarization depicted describes the magnetic (electric) polarization of free space that couples to $\psi$. Figure 7 therefore correctly predicts the polarization dependence seen in Fig. 1 for TE$_{X,B_2}$.

A more expedient method to generate the selection rules, however, is to determine the irreducible representations present in $V$ and then employ the direct product tables (see Appendix A, Fig. A 2(a) and A 2(b)) to immediately write the selection rules for all modes present at the $\Gamma$ point of the perturbed lattice. This is done by (1) finding the point group in common among $V$ and $\psi$, (2) writing the irreducible representations of each factor in that point group, and then (3) determining if the direct product $\Gamma_V \otimes \Gamma_\psi$ matches the irreducible representation of a free space polarization (which are reported for each relevant point group in Appendix A, Fig. A 2(c)).

The irreducible representations of $V$ can be found by conventional Group Theory methods if required, but are generally apparent by inspection. Figure 8 depicts the decomposition of $V$ for the same space group as Fig. 7.

The process is simplified by properly choosing $H^0$ such that $V$ transforms as simply as possible. For instance, in Fig. 7, $H^0$ is written as a circle with permittivity $\varepsilon$ shadowing a square cross oriented in the $x, y$ directions with permittivity $\varepsilon/2$, as shown in Fig. 8(a). It is then clear to see that the $V$ depicted obtains $H$ upon addition of $H^0$.

Next, $V$ can be decomposed into two portions, one (called $V_L$) with the periodicity of the unperturbed lattice, and one (called $V_X$, here) with the periodicity of the perturbed lattice (Fig. 8(b)). By the periodicity constraints outlined above, $V_L$ contributes only to the modes with the same periodicity (that is, modes at the $\Gamma$ point in the unperturbed lattice) while $V_X$ contributes only to the modes with the periodicity of the perturbed lattice (modes at the $X$ point in the unperturbed lattice). The point group of both $V_L$ and $V_X$ is the same as the point group of the space group, $C_{2v}^\mu$. Referring to the character table of $C_{2v}^\mu$ (Fig. 8(c) or Appendix A, Fig. A 1(a)), it is readily apparent that $V_L$ transforms as $A_1$ and $V_X$ transforms as $B_2$.

Finally, the coupling constraint (Eq. (18)) is evaluated. However, since the modes of interest are defined in a higher group than that of $V$, we must first determine how they degenerate into the lower group. This can be done by referring to the symmetry degeneration tables (see Appendix A, Fig. A 1(c)). Then, the direct products $\Gamma_V \otimes \Gamma_\psi$ are taken with reference to the direct product table for the point group $C_{2v}^\mu$. Since $x, y$ polarized planewaves transforms as $B_1, B_2$ in $C_{2v}^\mu$, the modes for which the product $\Gamma_V \otimes \Gamma_\psi = B_1, B_2$ couple to $x, y$ polarization, respectively. Figures 8(d) and 8(e) show a worksheet of this process. It bears repeating that this polarization corresponds to that of the out-of-plane field component. For example, if $\psi$ is a $H_z$ mode, then $x$ refers to the $H_x$ component of the free space planewave, corresponding to $y$ polarized light as conventionally defined by the electric field. The resulting selection rules are in agreement with the graphical method in Fig. 7, but required a single diagram to decompose $V$ instead of one for each mode, and straightforwardly give the selection rules for the $\Gamma$ point modes as well (for which the graphical method would require another set of diagrams).

The method detailed throughout this section may be summarized as follows. First, the unique space groups compatible with each lattice type are determined by exhaustion. Second, for each of these space groups, the perturbation is split into $V_T$ and $V_L$, where $L$ is the high symmetry point of the unperturbed reciprocal lattice that is folded to the $\Gamma$ point. Third, the irreducible representation of each portion of the perturbation is determined. Fourth, the coupling condition, Eq. (18), is evaluated for each mode, using $V_T$ for $\psi_{G,S}$ and $V_L$ for $\psi_{L,S}$; the matching polarization (if any) is marked down by reference to Fig. A 2(c).

With this method, a catalogue for each of the six lattice types is generated, for each of the compatible degenerated space groups described above. The catalogue for each lattice types are given in Fig. 9 for square lattices, and in Fig. 10 for hexagonal lattices. An entry of the catalogue lists the space group by name, the point group used to describe $V$, the irreducible representations of $V_T$ and $V_L$, an example visualization of the degenerated lattice (using the “keyhole” motif [58]), and the selection rules for all the modes present at the $\Gamma$ point in the perturbed lattice.

Note: the selection rules for the two-fold cyclic space group, $p2$, in the catalogue are specified by some angle, $\phi$ or $\theta$, which are ill-defined relative to the lattices’ axes: the polarization angle must be numerically determined, will generally change with the magnitude of the perturbation, and may differ between TM and TE modes of the same symmetry. However, for small perturbations, two modes specified by $\phi$ will be “correlated”, or excited by the same polarization angle $\phi$, whatever that may be; $\theta$ denotes the angle orthogonal to $\phi$. Note that the Group Theory approach in Fig. 8 can only say that some polarization couples, but cannot specify $\phi$ and $\theta$; for this, the diagrammatic approach in Fig. 7 is used. The selection rules for $p1$ are ill-defined in a similar way, but are not generally “correlated” in the same way, and are therefore specified as any. The remaining cyclic space groups, $p3$, $p1$, and $p6$, only allow access to degenerate modes in a polarization independent manner, and so for simplicity are specified as $x, y$.

**IV. DISCUSSIONS AND APPLICATIONS**

The process described above lays out the derivation of the selection rules for two-dimensional PCSs with in-plane perturbations applied. The resulting catalogue,
FIG. 9. Selection rules catalogue of the square lattices. As depicted by the legend, each entry specifies the space group, the point group, the irreducible representations of the two components of the perturbation, $V$, and the selection rules for each high symmetry mode. Example TM modes of each irreducible representation are shown for reference. Polarization directions are defined by the given axes. Colored squares and ovals denote points with four-fold and two-fold rotational symmetry, respectively.
FIG. 10. Selection rules catalogue of the hexagonal lattices. As depicted by the legend, each entry specifies the space group, the point group, the irreducible representations of the two components of the perturbation, \( \Gamma \), and the selection rules for each high symmetry mode. Example TM modes of each irreducible representation are shown for reference. Polarization directions are defined by the given axes. Colored stars, triangles, and ovals denote points with six-fold, three-fold, and two-fold rotational symmetry, respectively.
split into Figs. 9 and 10, contains a great amount of information and warrants further discussion and exploration. In particular, a few unique features present in the catalogue readily motivate device applications not possible in the simpler one-dimensional PCFs.

For instance, due to the two-dimensional nature of the device, the band structure can be optimized in both in-plane directions, allowing for full optimization of the band structure and thereby optimally compact devices. One-dimensional structures (e.g., devices composed of rectangular grating fingers, invariant in one in-plane direction) can be understood as a special case of a subsection of the $Sq_M$ lattice, but with limited to no control over the behavior along the direction of the grating fingers.

Additionally, the higher in-plane symmetry of two-dimensional structures means the presence of degenerate $E$-type modes ("partner" modes with identical eigenfrequencies that couple to orthogonal polarizations), which do not exist in one-dimensional structures. This allows for compact, polarization independent devices such as filters and modulators to be designed. The manipulation of degenerate modes is therefore of considerable technological interest. With this sort of application in mind, we consider here a number of interesting features and applications of the catalogue.

A. The Nature of Degenerate Modes

We first consider the nature of degenerate modes. The degenerate modes generally transform as partners of a degenerate irreducible representation (e.g., $E$ in $C_{4v}$), which are written $E^x$ and $E^y$ corresponding to their dipole moments. Because of this dipole moment, the $E^x$ and $E^y$ modes in the unperturbed $Sq_{4T}$ lattice generally couple to free space (and the $E_1$ modes couple in the unperturbed $Hex_T$ lattice). In other words, the integral

$$\int c_{m,n} \partial_1 \psi \, dx \, dy,$$

which has an integrand that transforms as $\Gamma_1 \otimes \Gamma_{\partial_1} \otimes \Gamma_{\psi}$, is non-vanishing for $E$ modes because $\Gamma_{\partial_1} = E$ in $C_{4v}$ (likewise, $\Gamma_{\partial_1} = E_1$ in $C_{6v}$). The coupling can numerically vanish for certain combinations of angle, polarization, and optical materials, but since these are reasons unrelated to the symmetry arguments above, they are accidental BICs. All modes other than the $\psi_{\Gamma,E}$ for $Sq_T$ and $\psi_{\Gamma,E_{1}}$ for $Hex_T$ in the mode classification are symmetry-protected. For the modes already coupled to free space in the unperturbed lattice, the only significant impact a perturbation has is to split the degeneracy upon symmetry degeneration (for instance, perturbing a lattice with $C_{4v}$ down to $C_{2v}$). In other words, if the lattice is made structurally birefringent, the $E^x$ and $E^y$ modes will degenerate into irreducible representations in a lower order point group with different eigenfrequencies, but the coupling rate will generally be changed to a negligible degree. For this reason, Figs. 9 and 10 simply label the corresponding entries $x,y$.

More interesting are the degenerate symmetry-protected BICs. The $M$ point modes of either square or hexagonal lattices have no such degenerate modes because the $C_{2v}$ point group has no degenerate irreducible representation (a rectangle is not identical in the $x,y$ directions). However, the $\psi_{\Gamma,E_2}$ for $Hex_T$, $\psi_{X,E}$ for $Sq_X$ and $\psi_{K,E_1}$ and $\psi_{K,E_2}$ for $Hex_K$ are degenerate symmetry-protected BICs. Therefore, a polarization insensitive filter or modulator must use one of these lattices in order to utilize the advantages of symmetry-protected BICs (that is, a Q-factor controllable by Eq. (1) independent of the band structure, following, for instance, the approach outlined in Ref. [50] for one-dimensional, polarization dependent devices). We consider the degenerate modes in each of these three lattices in turn.

The $Hex_T$ supports the $E_2$ modes, which are uncoupled to free space in the absence of a perturbation ($E_1 \otimes E_2 = B_1 + B_2 + E_1$, which does not contain $\Gamma_1$ in $C_{6v}$) and are therefore degenerate BICs. Reference to the catalogue shows that reducing the symmetry to $C_{3v}$ or lower may allow coupling to these modes. A polarization independent filter or modulator with Q-factor following Eq. (1) could be made utilizing the $E_2$ modes of a $Hex_T$ lattice using either the $p31m$ or $p3m1$ entry of the catalogue.

The $Sq_X$ lattice supports degenerate modes that are bound in the unperturbed lattice. Upon perturbation, they are brought to the $\Gamma$ point, allowing coupling to free space at normal incidence. Several space groups in the $Sq_X$ lattice leave these modes uncoupled in the continuum, making them BICs, while most others allow for coupling with a spectral feature obeying Eq. (1). The space groups with $C_4$ and $C_4$ leave the eigenfrequencies degenerate, while lower order symmetry groups have birefringent behavior. Therefore, a polarization independent filter or modulator with Q-factor following Eq. (1) may be made utilizing the $E$ modes of a $Sq_X$ lattice using any of the $p4m$, $p4g$, or $p4$ entries of the catalogue as reference.

An interesting feature of the catalogue is the prediction of coupling of the $E^x$ partner of the $E$ modes of a $Sq_X$ lattice to either $x$ or $y$ polarized light (equivalently, $y$ polarized light may couple into either the $E^x$ or $E^y$ partner). Compare, for instance, the $p4m$ (Fig. 11(a)) and $p4g$ (Fig. 11(b)) space groups in the $Sq_X$ lattice. Figure 11(c) and 11(d) depict, for the $p4m$ and $p4g$ cases respectively, the field profiles calculated by full-wave simulations at a resonance excited by $y$ polarized light (magnetically $x$ polarized light) at the frequency of the $TE_{X,E}^{1,1}$ modes. The former shows that the magnetically $x$ polarized light couples to the $E$ mode with the apparent dipole in the $y$ direction (that is, the $E^y$ partner, as defined in Fig. 7), while for the latter it couples to the $E$ mode with the apparent dipole in the $x$ direction (that is, the $E^x$ partner). This mode “twisting” is written in the cat-
are degenerate, despite the mode classification scheme in Fig. 2 predicting the presence of modes not describable by $E$ irreducible representations. In particular, the fundamental modes are degenerate, but have irreducible representations $A_1$ and $B_1$. Although visibly quite different (see the $K^{(1)}$ column of Fig. 4), and having distinct symmetries in $C_{6v}$, they are nonetheless identical in eigenfrequency. This degeneracy is born of the trimerization of the lattice: a pair of modes with the same eigenfrequency are superposed upon translation to the $Γ$ point, and can be superposed either in phase or out of phase, producing a pair of distinct modes with identical eigenfrequency. That is, in contrast to the $E_1$ and $E_2$ modes, the magnitudes and the directions of the planewaves composing the resulting modes are identical, but the phases are not.

One consequence of this is that in the $p31m$ $Hex_K$ lattice with point group $C_{6v}^d$, the $A_1$ and $B_1$ modes form a degenerate pair that together correspond to a spectral feature that is polarization insensitive (a similar behavior is seen in the $p3$ lattice where $V_K$ transforms as a partner of the $E$ irreducible representation). This reveals another way to consider this degeneracy: the $A_1$ and $B_1$ modes are partners of the $E$ irreducible representation of the $C_3^d$ point group, defined about the $κ$ point in the real space lattice (as defined in the $Hex_K$ lattice in Fig. 5). Because the $γ$ point has the full symmetries of $C_{6v}$, describing the modes about the $κ$ point misses relevant symmetries; nevertheless, the ability to describe them in $C_3^d$ as partners of the $E$ modes means their eigenfrequencies are identical. Upon further symmetry degeneration (for instance, to $cmm$, or $cm$ in the $Hex_K$ lattice), the modes behave differently, splitting in both eigenfrequency and polarization dependence. This behavior is unique to the $Hex_K$ lattice in Figs. 9 and 10 because it is the only lattice with more than two atoms per unit cell. Higher order lattices, such as those shown in Fig. B 1, may exhibit similar behavior.

B. Application: Terahertz Generation

We explore this feature of the degenerate fundamental modes of the $Hex_K$ lattice to aid in generating Terahertz (THz) frequencies through nonlinear processes enhanced by optical resonances. Sketching the design of such a device is a useful exercise to demonstrate the utility and an example use of the catalogue. Figure 12(a) depicts a schematic of the device, with a $Hex_K$ lattice made of Silicon pillars in the gap of a bowtie antenna resonant to a THz frequency. Figure 12(b) shows an example spectrum of the PCS portion of this device, showing two closely spaced resonances at $λ_1 = 3.147 \mu m$ and $λ_2 = 3.161 \mu m$, both excited by $y$ polarized light and associated with the split degeneracy of the $TE_{K,A_1}^{1,1}$ and $TE_{K,B_1}^{1,1}$ modes. If optical power is normally incident at pump wavelengths $λ_a$ and $λ_b$ such that $λ_a = λ_1$ and $λ_b = λ_2$, and a low-frequency bias (corresponding to a radiofrequency with wavelength $λ_3$) is electrically applied across the antenna,
four-wave mixing will produce photons at a THz wavelength with improved efficiency (compared to a bulk material) due to the enhanced light-matter interactions from the resonances and antenna geometry. The case shown in Fig. 12(b) corresponds to \( \lambda_4 = 711 \text{\mu m} \), but Fig. 12(c) shows that \( \lambda_4 \) can be easily tuned by the radius of the central pillar, \( R_1 \). Figure 12(d) confirms that the figure of merit (defined below) is indeed maximum at \( \lambda_4 \) when the pump photons have wavelengths of \( \lambda_1, \lambda_2 \) (1/\( \lambda_3 = 0 \) for simplicity; here, it may generally be used to finely and actively tune \( \lambda_4 \)).

A key advantage of using these degenerate modes is the unique robustness of the control of both the spectral spacing and linewidths of the resonances. Since the modes are degenerate in the unperturbed lattice, they are necessarily closely spaced in a weakly perturbed lattice. Then, by controlling the radius of one of the pillars, the frequency spacing can be finely tuned. The spectral map in Fig. 12(c) shows the impact of tuning the radius of the central pillar, \( R_1 \), depicting a classic anti-crossing behavior [39] as the resonance spacing changes. This utilization of degenerate modes offers considerably more robust control of closely spaced resonances compared to relying on “accidental” alignment of two unrelated resonances by tuning geometric parameters: an accidental resonance alignment is highly sensitive to fabrication errors, while the split degeneracy here is guaranteed by symmetry.

Notably, \( \lambda_4 \) (or the spacing of the resonances) can be tuned largely independently of the linewidths of the resonances. This is easily understood by considering the portion of the perturbation, \( V_1 \), that corresponds to changing \( R_1 \). Depicted in Fig. 12(e), a lattice perturbed by \( V_1 \) alone produces a \( H_{exK} \) lattice with the \( p6mm \) space group; reference to the catalog (Fig. 10) reveals that no coupling to the target modes is introduced by this perturbation. Tuning the radius of the central pillar therefore does not impact the coupling to first order. Then, the addition of \( V_2 \) degenerates the space group to \( cnmm \), which couples the TE\(_{K,B_1}^1 \) mode to the magnetic \( x \) polarization, but not the TE\(_{K,A_1}^1 \) mode. Finally, the addition of \( V_3 \) creates a lattice with the \( cm \) space group with \( C_s^\alpha \) point group, allowing coupling to TE\(_{K,A_1}^1 \) to the
magnetic $x$ polarization. Notably, if the other $cm$ space group (with point group $C^d_4$ in the third table of Fig. 10) were used, the two resonances would be cross-polarized. Tuning these three portions of the perturbation therefore allows independent tuning of each of the linewidths and the spacing of the two resonances in either a co-polarized or cross-polarized fashion. The co-polarization of the two previously degenerate resonances is unique to the $Hex_K$ lattice in the catalogue, as the $E_1$ and $E_2$ modes for the hexagonal lattices (and $E$ modes in the square lattices) are only accessible in a cross-polarized fashion. Co-polarized split degenerate states are a unique feature of lattices with more than two atoms (such as the lattices containing four atoms seen in, for instance, Fig. B1). In the present application, the freedom to have the pump wavelengths be co-polarized allows a single pulse (with bandwidth spanning the two resonances) as the pump.

To complete the demonstration of the unique advantages of the $Hex_K$ lattice for Terahertz generation, we compute a simple figure of merit related to the efficiency of this conversion (see, for instance, Refs. [22, 23]):

$$FoM = \int \int \chi^{(3)}(x, y) E^*(\omega_1) E(\omega_2) E^*(\omega_3) E^*(\omega_4) \, dx \, dy$$

where the bounds of integration are over the entire device and $\chi^{(3)}(x, y)$ is the spatially dependent third-order nonlinear susceptibility and the electric fields are normalized to the corresponding incident fields. Given the scale difference of $\lambda_3$ to a unit cell (i.e., $\lambda_3^3 \gg A$), a reasonable approximation to this integral is that $E^*(\omega_3) = F_3$ and $E^*(\omega_4) = F_4$ are constants equal to the electric field enhancement due to the bowtie antenna at each frequency. We may then integrate over a unit cell:

$$FoM = \left| \int_A \chi^{(3)}_{SI} F_3^* F_4^* \int_A F_y(x, y) \, dx \, dy \right|$$

where $F_y = E^*(\omega_1) E_y(\omega_2) G(x, y)$ and $G(x, y) = 1$ where there is Silicon and is 0 where there is vacuum. That is, the figure of merit is proportional to the overlap integral of the two pumps within the Silicon portion of a unit cell.

The integrand may be calculated from the mode profiles taken from full-wave simulations of unit cell of the device. The $H_2$ component of the modes for the spectrum in Fig. 12(h) are shown in Figs. 12(f) and 12(g), corresponding to the choice in Fig. 12(c) of $R_1 = 0.38 \mu m$. The integrand of Eq. (22) is shown in Fig. 12(h), as calculated from the $E_y$ components of the modes (seen in Figs. 12(i) and 12(j)) and the refractive index profile of the device. The numerical value for this case is $FoM/\chi_{SI}^{(3)} \approx 114 |F_3| |F_4|$, meaning for a modest enhancement of $\left|F_3\right| = |F_4| \approx 10$ by the bowtie antenna we will have a total enhancement of $FoM/\chi_{SI}^{(3)} \approx 10^4$ in efficiency. Figure 12 therefore demonstrates a platform to produce THz light from two infrared pumps taking advantage of large electric field enhancement at every frequency involved in the four-wave mixing process. The

FIG. 13. Mechanically tunable optical lifetime. (a) Schematic of a $Hex_K$ lattice with a $p6mm$ space group on a stretchable substrate. (b) Full-wave simulations mapping the spectral reflectance, $R$, near the wavelength, $\lambda$, of the $TE_{11}^{1.1}$ mode for various degrees of stretching. (c) The unstretched lattice, with spacing $P$. (d) Stretched lattice, with spacing $P'$ along the horizontal. Single sided arrows denote the lattice vectors in (c) and (d).

Finally, we remark on a type of periodic perturbation achieved by stretching or shearing a high symmetry lattice. Since the symmetry of the lattice is reduced, the symmetry-protected BICs may be excited. However, the condition on coupling (that is, Eq. (18)) still applies, and therefore this class of perturbation follows the same selection rules as the equivalent point group degeneration entries. For instance, by shearing an unperturbed $SqI$ lattices unit cell from a square into a rhombus, the space group is reduced to $p1$ and any mode at the $\Gamma$ point may now couple to free space with a strength related to the degree of shear. However, the polarization direction of the coupled planewave will be ill-defined in general, changing, for instance, with the degree of shear. (Recall that it is for this reason that the $p1$ entries are all specified as
Of more interest is stretching along a high symmetry axis, affording well-defined selection rules. This has been explored in Ref. [28] for plasmonic heptamers arranged in a square lattice by degenerating the symmetry of the heptamer from $C_{6v}$ to $C_{2v}$ by stretching the substrate. Since the Fano resonance in the plasmonic heptamer is both (1) well-confined to a unit cell of the overall lattice, and (2) due to the coupling between plasmonic modes, analysis of the point group of the unit cell alone suffices to analyze the resonance. However, for a low loss, high Q-factor demonstration using dielectric structures, this analysis is insufficient because the coupling across unit cells of the array is integral to the presence of BICs. The catalogue of selection rules derived here provides the necessary information for proper analysis in dielectric systems.

Inspection of the square catalogue reveals that square lattices afford no interesting cases: the only impact of a lattice deformation along a high symmetry axis is to split degeneracies, not introduce any new coupling. The same is not true for the hexagonal lattices, however. Figure 13(a) shows a $Hex_K$ lattice with $p6mm$ space group (one pillar of the trimer has a larger radius than the others) on a stretchable substrate. In the unstretched case, the lattice has $C_{6v}$ symmetry, and the selection rules forbid coupling to any but the $E_1$ modes at normal incidence. However, inspection of the $cmm$ lattice reveals that degeneration from $C_{6v}$ to $C_{2v}$ enables coupling to the $B_1$ and $B_2$ modes. Stretching the $Hex_K$ lattice with $p6mm$ space group along the $x$ axis also degenerates the point group from $C_{6v}$ to $C_{2v}$, and so ought to enable coupling to those modes to a degree controlled by the strength of the lattice deformation. Figure 13(b) depicts confirmation of this prediction via full-wave simulations near the TM$_{K,1}^{1,1}$ mode, showing redshift and a changing Q-factor as a function of deformation. Inspection of the $Hex_K$ catalogue (or an analogous case in the $Hex_T$ lattice) therefore motivates a low-loss dielectric-based flexible device platform with mechanically tunable optical lifetimes.

V. SUMMARY

We derive the selection rules for Fano resonances due to symmetry-protected bound states in the continuum supported in photonic crystal slabs. Targeting the high symmetry modes of both square and hexagonal lattices, we explore six lattices designed to bring each class of high symmetry mode into the continuum. We exhaustively report the degenerated space groups due to in-plane perturbations that are compatible with these six lattices, and catalogue the selection rules in each case by applying principles of Group Theory to determine the free space polarization of the leaky portion of the perturbed modes.

Together with band structure engineering, the principles, approach, and results outlined here provide a high-level guide to designing compact photonic crystal slabs supporting sharp resonances: devices confining light in both space and time, manufacturable by mature fabrication technologies. Future computational work will be well-guided by the symmetry constraints considered here to reduce the search space required to optimize a compact optical device. In particular, we show that the band structure may be engineered in the unperturbed lattice before a periodic perturbation is applied to couple the targeted mode(s) to the desired free space polarization(s). We also identify two novel phenomena from the symmetry-broken lattices explored here: (1) mode “twisting” and (2) co-polarized split degenerate states producing an anti-crossing. Lastly, our work motivates novel devices, such as polarization independent planar optical modulators, Terahertz generation in photonic crystal slabs with lifted degeneracies, and devices with mechanically tunable optical lifetimes.

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Appendix A: Group Theory Tables

For ease of reference, the character tables of all relevant point groups are reported in Fig.A 1(a). The left column of tables in Fig. A 1(a) contains the point groups compatible with the square and rectangle lattices, and the right contains those compatible with hexagonal lattices. Figure A 1(b) summarizes the subgroups of each of the point groups shown in Fig. A 1(a). This prescribes the necessary components of the symmetry degeneration tables, shown in Fig. A 1(c), which track how higher symmetry modes (irreducible representations) degenerate into lower groups. That is, reference to the symmetry degeneration tables provides the answers to how a higher symmetry
mode would be named in a lower order symmetry group (for instance, \( B_2 \) in \( C_{4v} \) would be called \( A'_1 \) in \( C_{2v} \)).

Next, Fig. A 2 provides the Group Theory tables helpful for determining the selection rules through the direct product approach. Figure A 2(a) provides the direct product table for the \( C_{6v} \) point group, and Fig. A 2(b) provides the same for the \( C_{4v} \) point group. The direct product tables for the lower order point groups are a subset of these. For instance, for \( C_{2v} \), Fig. A 2(b) may be used excluding the final row and column. Lastly, Fig. A 2(c) contains the irreducible representations for the partial derivative operators relevant for direct products such as in Eq. (18). This tracks how free space polarizations transform in each lattice type.

### Appendix B: Additional Lattices

The six lattices catalogued in Figs. 9 and 10 were chosen because they access the six high symmetry modes in the simplest way. For instance, the \( S_{qM} \) lattice accesses only the \( \Gamma \) and \( M \) (but not the \( X \)) modes of a square lattice, while the \( S_{qX} \) accesses the \( \Gamma \) and \( X \) (but

### FIG. A 1. Group Theory table for point groups. (a) The character tables of the point group relevant to the square (left) and hexagonal (right) lattices. (b) The subgroups of the higher symmetry lattices. (c) The symmetry degeneration tables, describing how irreducible representations in higher order groups degenerate in lower order groups.

![Character tables](image)

![Subgroups](image)

![Symmetry Degeneration](image)
FIG. B 1. Three additional examples of periodically perturbed lattices. Each of these lattices is a "quadromer" lattice, having four atoms per unit cell upon perturbation, and therefore have four times the modes of the unperturbed lattices at the Γ point.

Also pictured in Fig. B 1 are the $Hex_{MMM}$ and $Hex_{MA}$, both of which are examples of quadromer lattices. $Hex_{MMM}$ is still of the hexagonal lattice family, while $Hex_{MA}$ (much like $Hex_M$) is rectangular. $Hex_{MMM}$ contains three copies of the $M$ modes, which will mix at the Γ point. $Hex_{MA}$, on the other hand, accesses a unique set of modes at the Λ point in the unperturbed FBZ (see the last panel in Fig. B 1), which have the point group $C_d$ (that is, they are either symmetric or anti-symmetric about the x axis).

The lattices shown in Fig B 1 are by no means the only additional lattices that may be explored. Instead, they serve as an example of the next few lattices in the infinite list of lattices ordered by number of atoms in the perturbed unit cell. The lattices in this list are generally increasingly complicated, but the same approach outlined in Sec. III C may be applied to determined the selection rules if desired.