Symmetries and wave functions of photons confined in three-dimensional photonic band gap superlattices

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We perform a computational study of confined photonic states that appear in a three-dimensional (3D) superlattice of coupled cavities, resulting from a superstructure of intentional defects. The states are isolated from the vacuum by a 3D photonic band gap, using a diamondlike inverse woodpile crystal structure, and they exhibit "Cartesian" hopping of photons in high-symmetry directions. We investigate the confinement dimensionality to verify which states are fully 3D-confined, using a recently developed scaling theory to analyze the influence of the structural parameters of the 3D crystal. We create confinement maps that trace the frequencies of 3D-confined bands for select combinations of key structural parameters, namely the pore radii of the underlying regular crystal and of the defect pores. We find that a certain minimum difference between the regular and defect pore radii is necessary for 3D-confined bands to appear, and that an increasing difference between the defect pore radii from the regular radii supports more 3D-confined bands. In our analysis, we find that their symmetries and spatial distributions are more varied than electronic orbitals known from solid-state physics. We surmise that this difference occurs since the confined photonic orbitals derive from global Bloch states governed by the underlying superlattice structure, whereas single-atom orbitals are localized. Based on this realization, we suggest that the extent symmetries of "photonic orbitals" could possibly translate to novel macroscopic behaviors of "photonic solid-state matter," never before seen in the standard electronic solid-state systems. We also discover pairs of degenerate 3D-confined bands with p-like orbital shapes and mirror symmetries matching the symmetry of the superlattice. Finally, we investigate the enhancement of the local density of optical states for cavity quantum electrodynamics applications. We find that donorlike superlattices, i.e., where the defect pores are smaller than the regular pores, provide greater enhancement in the air region than acceptorlike structures with larger defect pores, and thus offer better prospects for doping with quantum dots and ultimately for 3D networks of single photons steered across strongly coupled cavities.

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I. INTRODUCTION

The confinement of light is a prominent goal of nanophotonics that is traditionally achieved via a single resonator that stores photons for a given time duration before they leak away to the surrounding vacuum [1–3]. All over the world, a large variety of resonator structures has been realized including micropillars [4,5], microdisks [6,7], rings [8,9], plasmonic resonators [10,11], and defects in one-dimensional [12–14] and two-dimensional photonic crystals [15–17] as well as three-dimensional (3D) photonic band gap crystals [18–24]. Light confinement in a single cavity has been

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practically utilized in applications ranging from sensing [25,26] and enhancing absorption [27], to slowing down or trapping of photons [28,29], and to enhancing spontaneous emission [4,30] and other cavity quantum electrodynamic (cQED) phenomena [5,6,31–34].

Novel physical opportunities arise when *multiple coupled* cavities are embedded in 3D photonic band gap crystals, as these crystals are capable of confining light in all three dimensions simultaneously [35–37]. In a perfect photonic crystal structure, thanks to multiple wave interference [38], the periodic translational symmetry gives rise to a 3D photonic band gap [39-42], that is, a range of frequencies for which light is forbidden to propagate inside the crystal irrespective of its wave vector and polarization. The introduction of intentional defects on a lattice superperiodic over the crystal lattice disrupts the local symmetry of the crystal, resulting in the appearance of a variety of localized states inside the band gap [35,36]. Some of these states give rise to so-called *Cartesian light* [35], whereby photons confined in one cavity in all three directions simultaneously hop to a nearby cavity, as described by the well-known tight-binding approximation

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FIG. 1. 3D superlattice of defect pores embedded as photonic dopants in a 3D inverse woodpile photonic band gap crystal. For certain defect states, confined photons hop between neighboring cavities in Cartesian directions, known as *Cartesian light*.

[43]; see Fig. 1. As a result, defect bands arise, analogous to coupled atomic orbitals that may hybridize in an atomic superlattice to become semiconductor defect bands that are notably pursued for photovoltaics [44]. 3D-confined states in superlattice structures have also great potential for cavity QED and Anderson localization of light.

A large bandwidth of the photonic band gap is a crucial factor to effectively shield the 3D superlattice states from the surrounding vacuum states [45], and to make the photonic cavity superlattice robust with respect to unavoidable fabrication disorder [46]. Exceptionally wide band gaps are known to occur in crystals with diamondlike symmetry [47]. An example of these are the so-called inverse-woodpile photonic crystals, consisting of two arrays of nanopores [48]. These structures have been realized using various nanofabrication techniques and high-index backbones [49]. In the Complex Photonic Systems (COPS) chair at the University of Twente, we have developed CMOS-compatible nanofabrication methods to fabricate such crystals by etching deep pores into silicon [50-54]. The cavity in these crystals is realized by altering the radius of two proximate orthogonal *defect* pores, thereby creating an excess of one type of material in their proximal region [23].

Inverse woodpile photonic crystals with and without defects have been investigated both theoretically [23,27,35,46,55,56] and experimentally [37,49,57–60]. To properly interpret the experimental data and provide guidance for fabrication, it is crucial to understand the dependence of the physical and optical properties of the crystal on its structural parameters, notably on the regular and defect nanopore dimensions. In recent work [36,61], we have developed an accurate methodology to analyze defects in (photonic) superlattices based on finite-size scaling and enhanced by unsupervised machine learning. Therefore, in this paper we apply the methods from Refs. [36,61] to perform a thorough



FIG. 2. (a) Structure of the perfect inverse woodpile photonic crystal. We employ a tetragonal unit cell with lattice constants *b* and *a*, and the pore radius *R*. A $2 \times 2 \times 2$ supercell is depicted. (b) Design of a cavity. The radius of two proximal defect pores (shown in green) is altered, resulting in a region with excess silicon or air, which behaves as a cavity that confines photons (orange glow). (c) *y*-*z* cross-section of the defect from the computational model for regular pore radius R = 0.24a and defect pore radius R' = 0.5R. Note that the *x*-*y* cross-section is identical due to the crystal symmetry. (d) *x*-*z* cross-section for the same pore radii as in (c).

computational characterization of light confined in 3D photonic band gap superlattices with respect to both pore sizes. We create so-called confinement maps by keeping one of the radii constant while varying the other one and mapping the frequencies of confined photon bands. We analyze the symmetry of selected bands and investigate the enhancement of the local density of states (LDOS) [2,62] that is crucial for future applications in cQED [33] and quantum information processing (QIP) [63].

II. METHODOLOGY

We study 3D cavity superlattices embedded in 3D inverse woodpile photonic band gap crystals. The inverse woodpile crystal structure consists of two perpendicular arrays of nanopores with radius *R* in a high-refractive-index medium such as silicon [48], as illustrated in Fig. 2(a). In our computations, we use the relative permittivity $\varepsilon = 12.1$ to model silicon in the relevant near and short-wavelength infrared (NIR, SWIR) spectral range that includes the well-known telecom bands [46,55,56].

The plane normal to each pore array corresponds to the (110) crystal face of a conventional diamond structure. We employ a tetragonal unit cell with lattice parameters *b* (in the *x*- and *z*-directions) and *a* (in the *y*-direction). We set $a/b = \sqrt{2}$ to ensure a cubic crystal structure. Varying the ratio R/a results in tuning of both the center frequency and the bandwidth of the band gap, as shown in Fig. 3. It has been found that the widest band gap is obtained for the ideal radius R/a = 0.245 [46,55]. Throughout this paper, we express all frequencies as a reduced frequency $\tilde{\omega} = \omega a/(2\pi v)$, with *v* the



FIG. 3. Band gap frequencies as a function of pore radius *R* in an inverse woodpile photonic crystal with $\varepsilon = 12.1$ typical for a silicon backbone. The 3D photonic band gap exists for pore radii $0.15 \le R/a \le 0.29$, with the maximum width at R/a = 0.245.

speed of light in vacuum, to apply our results to any spectral range, e.g., from microwaves via optics to x-rays.

We introduce a single cavity in an inverse woodpile photonic crystal by altering the radius $R' \neq R$ of two proximate perpendicular *defect pores* [23], as shown in Fig. 2(b) and in the cross-sections in Figs. 2(c) and 2(d).¹ We introduce multiple cavities by introducing defect pores at every third pore of the underlying inverse woodpile structure, giving rise to a defect superlattice of linear size N = 3 that is commensurate with the underlying crystal. The introduction of the defect superlattice causes some of the bands to move into the band gap of the perfect crystal. The states of these defect bands are then confined in various dimensions, depending on the structure of the defect. We denote the number of dimensions in which a band of states is confined as the *confinement dimensionality c*. For more discussion on defect superlattices and wave confinement dimensionalities, see Ref. [36].

In this paper, we aim to find point-confined (c = 3) bands and investigate their dependence on the structural parameters of the inverse woodpile photonic crystal. To this end, we employ the scaling analysis of Ref. [36], supplemented by the MBC clustering algorithm presented in Ref. [61]. Specifically, we utilize the scaling to identify the set of confinement dimensionalities c present in the structure, which is then supplemented as an input to the MBC clustering algorithm. Note that for small supercells, the scaling analysis tends to identify several bands as plane-confined (c = 1), which is unphysical since our superlattice does not contain plane defects. We thus automatically exclude the c = 1 confinement dimensionality from the input into the MBC algorithm. We note that, even though the power of this analysis method exceeds any other known method of confinement classification, it is known to be



FIG. 4. Band structure of an inverse woodpile cavity superlattice with regular pore radius R = 0.24a and defect pore radius R' = 0.5R. Bands that are identified to be confined in c = 3 dimensions are colored, with red designating individual bands and blue indicating pairs of degenerate bands. Note that the degeneracies can be properly identified only after the qualitative discussion in Sec. IV. The colored bands are also labeled by their band number N_b . The inset shows the tetragonal Brillouin zone with labeled high-symmetry points.

not fully accurate for small supercells [36], so a few out of many bands may end up being misidentified, as will also be discussed later on.

Our confinement analysis requires knowledge of the energy-density distribution $W(\mathbf{r})$ in the superlattice. We have calculated the energy densities as functions of the crystal pore radius R/a and the defect pore radius R'/R using the plane-wave expansion method implemented in the MPB code [64]. We normalize the density for each band so that $\int_{V_S} W dV = 1$. The band structures have been computed using the MPB code as well. For applications in spontaneous emission control, we also investigate the maximum energy density of each band, defining $\Omega := \max_{V_S} W(\mathbf{r})$. A high Ω then corresponds to a high concentration of energy in the cavity and thus to an enhanced LDOS. To obtain the isosurface plots, we employ MATLAB's *isosurface* function to calculate the isosurface corresponding to one-third of the maximum of the energy density $W(\mathbf{r}) = \Omega/3$ as a representative gauge.

III. PHOTONIC STATES BEYOND ATOMIC ORBITAL ANALOGIES

Here, we investigate the spatial energy-density profiles of several salient bands of confined states in the superlattice with dimensions R = 0.24a and R' = 0.5R. As we will see, the main results are readily generalized to photonic superlattices in general. Some useful properties, such as band degeneracies, are best observed from the photonic band structure. Figure 4 shows the band structure of an inverse woodpile crystal with pore dimensions R = 0.24a, R' = 0.5R. The lower edge of the bulk 3D photonic band gap occurs at reduced frequency $\tilde{\omega} = 0.49$ [35], and states below this frequency are Bloch modes that freely propagate through the whole crystal volume in

¹Note that permittivity maps $\epsilon(\mathbf{r})$ reveal also values between those of air and silicon [$\epsilon_{air} \leq \epsilon(\mathbf{r}) \leq \epsilon_{Si}$] in our binary air-Si structure due to an inherent smoothening in the employed MPB numerical method that serves to enhance its accuracy; see Ref. [64] for details.

any possible direction. Inside the band gap, multiple confined defect bands occur. We label the bands by their band number N_b that is assigned in increasing frequency order. The bands that are identified to have c = 3 confinement are colored in red and blue to be easily recognizable. As an exemplary Cartesian band, we analyze the energy-density distribution of band $N_b = 111$ that was previously investigated in detail in Refs. [23,27,35] (where it was labeled as an m = 3 superlattice band). Reference [27] concluded, also on the basis of the data of Ref. [23], that the wave functions of this band have a quadrupolar symmetry, analogous to a 3*d* electronic orbital.² Below, we discuss that drawing such an analogy between photonic and atomic orbitals is misleading and that the inverse woodpile photonic structure in fact presents a new challenge in symmetry description.

Figure 5(a) shows a 3D view of the energy-density distribution $W(\mathbf{r})$ of the $N_{\rm b} = 111$ band whose states are confined within the cavity created by the crossing defect pores. One can immediately see that the symmetries are strongly influenced by the defect-pore symmetry shown in Fig. 2(b). There is a high-energy-density volume centered around x/b =1.5, y/a = 1.15, z/b = 1.5. The volume is divided by the $y/a \approx 1.15$ plane into two half-spaces, where it contains a dent in each of these half-spaces. For y/a < 1.15, the dent is along the x-direction and is surrounded in the same half-space by two smaller regions at both z/b < 1.5 and z/b > 1.5. For y/a > 1.15, the second dent in the central volume spreads in the z-direction and is surrounded by two smaller regions at both x/b < 1.5 and x/b > 1.5. The energy-density profile exhibits mirror symmetries along the $z/b \approx 1.5$ and $x/b \approx 1.5$ planes, but not along any plane of constant y/a, similar to the structure of the parent superlattice.

From the view in Fig. 5(a), it is clear that the energy density does not have the quadrupolar symmetry as in a 3d electronic orbital, since it lacks the 90° rotational symmetry characteristic for such a 3d electronic orbital [43]. Moreover, we argue that the actual symmetry of the photonic states differs remarkably from that of an atomic 3d orbital. Therefore, we show in Fig. 5(b) the 2D view of the energy density for the same $N_{\rm b} = 111$ band from the *y*-*z* plane. From this view, it is apparent that the confined states exhibit a combined mirrorrotation symmetry, namely mirror symmetry with respect to the plane $y/a \approx 1.15$ combined with a 90° rotation about the $(x/b, z/b) \approx (1.5, 1.5)$ axis. We attribute this result to the fact that the confined photonic orbitals derive from extended Bloch states that are governed by the underlying superlattice structure, whereas electronic orbitals in atomic superlattices derive from localized atomic orbitals.

This discovery brings us to an extremely interesting fundamental question: Instead of striving for strict analogies in symmetries between electronic and photonic orbitals, photonic structures could be utilized to create photonic "orbitals" with a much greater variety of geometries and symmetries than are feasible in spherical atoms [65] and controllable in more complicated electronic systems. Since there is a great



FIG. 5. 3D isosurface of the energy density [at $W(\mathbf{r}) = \Omega/3$] for confined band $N_b = 111$ in an inverse woodpile cavity superlattice with regular pore radius R = 0.24a and defect pore radius R' = 0.5R. The energy profile exhibits specific symmetries inherited from the parent defect superlattice. Besides the mirror symmetries along the $z/b \approx 1.5$ and $x/b \approx 1.5$ planes, it is also symmetric with respect to mirroring according to the $y/a \approx 1.15$ plane combined with 90° rotation about the $(x/b, z/b) \approx (1.5, 1.5)$ axis. (a) Birds-eye view; (b) view from the y-z plane.

diversity of photonic crystals of various structures and a plethora of options to introduce defects of different kinds in them (see, e.g., Refs. [41,47]), it is highly plausible that the set of symmetries achievable by "photonic orbitals" could be much more numerous and varied than the ones occurring in electronic orbitals. Since it is well known from atomic solidstate physics that the symmetries of atomic orbitals are closely tied to the appearance of the band structure and even to the macroscopic behavior of materials, such as their placement in the Periodic Table [43], it is exciting to investigate to what extent the symmetries in "photonic orbitals" translate to the macroscopic behavior of "photonic solid-state matter" and how their great variety can be utilized.

IV. SYMMETRY AND DEGENERACY

Figure 6 shows the *x*-*z* view of the energy-density distribution $W(\mathbf{r})$ of all nondegenerate c = 3 (3D) confined bands $N_{\rm b} = 111-115$ and 118 from the band structure in Fig. 4. All bands shown appear to have unrelated spatial energy-density distributions, which agrees with the fact that these bands are

²Note that lowercase "3d" refers to the electronic orbital and should not be confused with capitalized "3D," which stands for "three-dimensional."



FIG. 6. The *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] of nondegenerate 3D-confined bands in an inverse woodpile cavity superlattice with regular pore radius R = 0.24a and defect pore radius R' = 0.5R. While this view may convey the suggestion of a 90° rotational symmetry in these distributions, this is not the case, as may be verified by comparing to Fig. 5 for the $N_{\rm b} = 111$ band.

nondegenerate. Even though they appear to have 90° rotational symmetries, this is an optical illusion created by the in-plane view of the distributions, as is readily seen by comparing the appearance of the band $N_b = 111$ in Fig. 6 with the bird's-eye view of the same band in Fig. 5(a). It is important to emphasize that these distributions exhibit mirror symmetries with respect to the x/b = 1.5 and z/b = 1.5 planes, which both pass through the axes of each defect pore. We also note that the confined $N_b = 118$ band appears to be degenerate with the $N_b = 119$ band, which is not identified to be confined. This quasi-paradox is likely due to the decreased accuracy of the employed scaling method for small supercells, as previously described in detail by us in Refs. [36,61].

Figure 7 shows the energy-density distribution $W(\mathbf{r})$ for two pairs of degenerate bands $N_{\rm b} = 109, 110$ and 116, 117. These bands are related to each other by the mirror symmetries along the planes $x/b \approx 1.5$ and $z/b \approx 1.5$. In



FIG. 7. The *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] of the degenerate pairs of 3D-confined bands in an inverse woodpile cavity superlattice with regular pore radius R = 0.24a and defect pore radius R' = 0.5R. The dashed lines indicate the planes of the mirror symmetry between these pairs of bands, and the red circles for the bands $N_b = 116$, 117 indicate where the mirror symmetries are easily spotted.

solid-state physics, atomic orbitals are categorized as different spherical multipoles [43]. This is possible due to the spherical symmetry of the atomic geometry, with each multipole exhibiting a lower symmetry than spherical symmetry. One thus obtains three mutually orthogonal dipoles, each exhibiting a 180° rotational symmetry along every plane. Whereas the inverse woodpile structure obviously does not possess spherical symmetry, it possesses lower symmetry, namely only the x-z plane is rotationally symmetric with respect to 180° . This symmetry thus only allows for two mutually orthogonal dipoles, which are both symmetric with respect to 180° rotation in the x-z plane. Indeed, this symmetry is exhibited by the band pairs $N_b = 109, 110$ and 116, 117. We therefore interpret these two pairs of degenerate bands to be generalized dipoles for the case of the inverse woodpile structural symmetry. Moreover, within the limited set of the energy-density profiles that we have visually investigated, it seems that if the energy-density profile of a band is not symmetric with respect to both the mirror planes x/b = 1.5 and z/b = 1.5, the band turns out to be degenerate with another band that complements these mirror symmetries. This symmetry relation could therefore be used to spot or confirm the presence of degenerate bands in the inverse woodpile photonic band structure and likely be generalized to other situations and 3D structures.

We note that it may in practice be difficult to determine band degeneracies from the band structure only, due to, e.g., numerical noise. As an example, the bands $N_b = 114$ and



FIG. 8. The *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] of the Cartesian $N_b = 111$ band in an inverse woodpile cavity superlattice with varying regular pore radius *R* and constant defect pore radius R' = 0.5R.

115 exhibit a certain overlap in the band structures in Fig. 4, similar to the degenerate bands $N_{\rm b} = 116$ and 117. Only when inspecting the field profiles of these bands, as in Fig. 6, does it become clear that the bands are independent of each other. Therefore, only after a detailed examination of both the band structure and the mode profiles can one conclusively identify whether bands are truly degenerate, and color them in the band structures as in Fig. 4. Figure 8 shows the evolution of the $N_{\rm b} = 111$ band in structures with increasing pore radii R, while maintaining the ratio R'/R. The energy-density maximum of the band changes with increasing R, which makes it difficult to plot the same isosurface every time. Nevertheless, the mode seems to maintain a similar symmetric profile shape with strongly varying pore radius. This visualization confirms the results from Fig. 15 below, i.e., that for the radii R = 0.15aand 0.27*a* this band is not 3D-confined, since in both cases the profile extends throughout the whole supercell, at least in the x-z plane. It is remarkable that even for R = 0.27a, the shape of the central volume still resembles the confined profile seen for smaller radii. Overall, Fig. 8 offers the interesting

observation that, for a given band, its energy-density profile is robust to strongly varying structural parameters of the underlying inverse woodpile structure.

V. ENHANCED LOCAL DENSITY OF STATES AND CAVITY QED

It is well known that in thermodynamic equilibrium, the time-averaged energy density $\overline{W_{\omega}}$ of the electromagnetic field at frequency ω corresponds to the product of the average energy per mode $\overline{w}(\omega, T)$ and the local density of states (LDOS) $N(\mathbf{r}, \omega)$:

$$\overline{W_{\omega}(\mathbf{r},\omega)} = \overline{w}(\omega,T)N(\mathbf{r},\omega), \tag{1}$$

where *T* is the temperature; see, e.g., Ref. [2]. Expression (1) indicates that by manipulating the energy density *W*, we control the LDOS, which is a crucial control mechanism in cQED [2]. A large LDOS is favorable for cQED applications, initially for enhanced spontaneous emission and eventually, at even larger LDOS, for cQED strong coupling whereby quantum matter states are hybridized with photonic states [5,6,30,32,34,66,67]. By positioning quantum dots within the pores of inverse woodpile photonic crystal superlattices [68] and coupling them at the correct electromagnetic frequencies, it will be feasible to observe these cQED phenomena. It is therefore important to investigate the energy-density and LDOS enhancements of inverse woodpile cavity superlattices in response to their structural parameters.

As discussed below in Sec. VI in Figs. 11–15, it appears that larger pore radii R are generally more favorable towards confining light with large local enhancements of the optical energy density. Out of all investigated bands, $N_b = 108$ in the case of the R = 0.27a, R' = 1.2R structure has the largest maximum energy density equal to $\Omega = 29.6$. We therefore investigate the energy profile of this acceptorlike band in greater detail.

Figure 9(a) shows the cross-section of the permittivity of the investigated structure in the plane y/a = 1 for reference. Figure 9(c) then shows the energy-density distribution W of band $N_{\rm b} = 108$ in the same plane. To investigate the energy density more quantitatively, we plot W along the red line at (x/b, y/a) = (1.23, 1), resulting in the cross-section shown in Fig. 9(e). Figure 9(e) also shows the energy density for extended states (band $N_{\rm b} = 54$) for reference, to establish the vacuum energy density level by inspecting W in the air regions, from which we derive the vacuum energy density to be around W = 0.03. From this cross-section, it is clear that the band $N_{\rm b} = 108$ has large energy-density peaks, but these are restricted to the regions of high permittivity. In the central cavity region, the distribution of W within the large pore varies considerably and is an order of magnitude greater at the pore walls than at the pore center. Taking into account that quantum dots embedded in an inverse woodpile crystal may stick to the silicon walls, this structure could provide an LDOS enhancement of around one order of magnitude compared to the vacuum level. Nevertheless, overall it appears that the lack of silicon and air regions that are too large significantly restrict the energy density distribution in the acceptorlike structure, thus making it a sub-par candidate for cQED applications.



FIG. 9. Energy enhancement in two different inverse woodpile structures. (a), (c), (e) Acceptorlike structure with regular pore radii R = 0.27a, defect pore radii R' = 1.2R, band number $N_{\rm b} =$ 108. (b), (d), (f) Donorlike structure with regular pore radii R =0.26*a*, defect pore radii R' = 0.5R, band number $N_b = 109$. (a) Permittivity distribution of the acceptorlike structure in the y/a = 1plane. (b) Permittivity distribution of the donorlike structure in the y/a = 1.13 plane. (c) Energy density distribution of the acceptorlike band $N_{\rm b} = 108$ in the y/a = 1 plane. (d) Energy density distribution of the donorlike band $N_{\rm b} = 109$ in the y/a = 1.13 plane. (e) Cross-section of the energy density distribution for the (x/b, y/a) =(1.23, 1) line, denoted by the red line in (c). Depicted is the confined band $N_{\rm b} = 108$ and a reference extended band $N_{\rm b} = 54$. (f) Cross-section of the energy density distribution for the (x/b, y/a) = (1.60, 1.13) line, denoted by the red line in (d). Depicted is the confined band $N_{\rm b} = 109$ and for reference the extended band $N_{\rm b} = 54$.

To observe the influence of donorlike structures with R' <R on the energy density enhancement, we investigate the band $N_{\rm b} = 109$ in the superlattice with regular pore radius R = 0.26a and defect pores R' = 0.5R, which exhibits the maximal energy density $\Omega = 25.7$, which is the largest among the donorlike structures we studied. The permittivity distribution of this structure in the plane y/a = 1.13 is shown in Fig. 9(b) and the energy density distribution of confined band $N_{\rm b} = 109$ in the same plane is shown in Fig. 9(d). Figure 9(f) shows the energy density distribution along the red line in Fig. 9(d), given by (x/b, y/a) = (1.60, 1.13). We show also the energy density distribution for extended states (in band $N_{\rm b} = 54$) for reference. In this case, since the air volume is much smaller compared to the amount of silicon around the cavity, the energy density within the central defect pore is only slightly less than the high-energy density in the surrounding



FIG. 10. Band structures and mode profiles pertaining to our study of energy density and LDOS enhancement in 3D inverse woodpile cavity superlattices. (a) Band structure for regular pore radius R = 0.27a and defect pore radius R' = 1.2R with the studied band $N_b = 108$ marked in red. (b) Band structure for regular pore radius R = 0.26a and defect pore radius R' = 0.5R with the studied band $N_b = 109$ marked in red. (c) *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] for band $N_b = 108$, for regular pore radius R = 0.27a and defect pore radius R' = 1.2R. (d) *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] for band $N_b = 108$, for regular pore radius R = 0.27a and defect pore radius R' = 1.2R. (d) *x*-*z* plane view of the energy-density isosurface [at $W(\mathbf{r}) = \Omega/3$] for band $N_b = 109$, for regular pore radius R = 0.26a and defect pore radius R = 0.26a and defect pore radius R' = 0.26a and defect pore radius R' = 0.26a and defect pore radius R' = 0.26a and defect pore radius R = 0.26a and defect pore radius R = 0.26a and defect pore radius R = 0.26a and defect pore radius R' = 0.26a and defect pore radius R = 0.26a and defect pore radius R = 0.26a and defect pore radius R' = 0.6.

high-index silicon backbone. Overall, even at the center of the defect pore where W shows a local minimum, the energy density is more than two orders of magnitude greater than the vacuum energy density that is equal to W = 0.01. Therefore, the LDOS is two orders of magnitude enhanced compared to the vacuum LDOS. For completeness, the band structures containing the bands studied in this section as well as their mode profiles are illustrated in Fig. 10. To conclude the discussion on the enhanced LDOS, we observed three competing phenomena with regard to cQED applications: First, donorlike cavities are preferable for cOED due to larger silicon and smaller air regions. Second, as explained below in more detail, larger defect pore deviations, i.e., smaller defect pore radii R' for donorlike structures, favor the appearance of a larger number of strongly confined bands. Third, larger defect pore radii R' appear to favor more concentrated energy density. From our investigation it therefore seems that a good balance between these three requirements could occur around the defect pore radius $R' \approx 0.6R$, slightly above half the regular pore radius R.

VI. CONFINEMENT MAPS

A. Confinement versus defect pore radius

Figure 11 shows the confinement map of c = 3 pointconfined bands in an inverse woodpile superlattice with regular pore radius R = 0.24a while varying the radii R' of



FIG. 11. Confinement map of point-confined c = 3 bands in an inverse woodpile cavity superlattice with regular pore radius R = 0.24a and varying defect pore radii R'. The perfect crystal case occurs at R'/R = 1 as denoted by the dashed vertical line. Each point represents the average reduced frequency of a point-confined band, and the dashed red lines represent the edges of the band gap of a perfect crystal. The color and shape of the symbols correspond to their maximum energy densities Ω , as given in the legend.

the defect pores. We observe four salient features: First, there is a threshold in the defect pore radius, that is, a certain minimal deviation of the defect pore radius from the regular one necessary for the 3D-confined bands to be present. In this case, this threshold appears to be $R' \leq 0.8R$ or $R' \geq 1.2R$.

Second, we observe that for R' < R, the confined bands descend into the band gap from its upper band edge, while for R' > R, the confined bands ascend from the lower band edge. This notion agrees with the analysis of Ref. [69] and with the semiconductor analogy, where R' < R corresponds to donor doping while R' > R is analogous to acceptor doping [43]. In the photonic case, we interpret this behavior using the energy functional

$$\mathcal{U}(\mathbf{E}_{\mathbf{k}}) = \frac{\int_{V_{\mathbf{k}}} |\nabla_{\mathbf{k}} \times \mathbf{E}_{\mathbf{k}}|^2 \mathrm{d}V}{\int_{V_{\mathbf{k}}} \varepsilon |\mathbf{E}_{\mathbf{k}}|^2 \mathrm{d}V},$$
(2)

where $\nabla_{\mathbf{k}} \coloneqq \nabla + i\mathbf{k}$, V_{S} denotes the superlattice volume, and $\mathbf{E}_{\mathbf{k}}$ is the periodic part of a specific band mode at wave-vector **k**. It is known that each higher-frequency mode $\mathbf{E}_{\mathbf{k}}$ minimizes the functional $\mathcal{U}(\mathbf{E}_{\mathbf{k}})$ in the space orthogonal to all the lowerfrequency modes; see Ref. [41]. Decreasing the size of the defect pores R' < R results in additional high-index silicon in the crystal, which allows for a proportionally larger concentration of the electromagnetic energy inside the high-index material, thus lowering the minimum of the energy functional for the given mode and ultimately pushing the bands from the top of the band gap downwards. On the other hand, increasing the size of the defect pores R' > R results in more air in the structure and thus restricts the freedom of concentrating the energy in the high-index material for the bands below the band gap, thereby pushing them upwards into the gap. In this regard, it is also relevant that larger deviations of the defect pore radius R' from the regular pore radius R provide more 3D-confined bands.



FIG. 12. Confinement map of point-confined c = 3 bands in an inverse woodpile superlattice with regular pore radius R = 0.27a and varying defect pore radii R'. The unperturbed crystal occurs at R'/R = 1 as denoted by the dashed vertical line. Each point represents the average reduced frequency of a point-confined band and the dashed red lines represent the edges of the band gap of an unperturbed crystal. The color and shape of the symbols correspond to their values of maximum energy density Ω , as described in the legend.

Third, the confined bands exhibit a clear upward moving trend with increasing R'/R, until they disappear in the top edge of the band gap, creating groups separated by frequency gaps. It is worth noting that even though there are more confined bands for small defect pore sizes, only the large enough defect radii $R' \ge 0.3R$ provide the value of $\Omega > 10$, corresponding to large energy concentration.

Fourth, these confined bands do not abruptly disappear at the edges of the band gap, but sometimes extend slightly beyond them; specifically, some confined bands cross the bottom edge of the gap for R' < R, whereas certain bands cross the top gap edge for R' > R. This may be understood because the decrease of the defect pore radius increases the total silicon volume fraction of the underlying photonic band gap crystal, thus effectively shifting the whole band structure slightly down for R' < R, whereas the opposite happens for R' > R, where the lower silicon volume fraction shifts the band structure slightly up.

We note that the specific case of R = 0.24a, R' = 0.5R was previously investigated by means of a naive band-structure analysis by Refs. [23,27,35], all of which found only five 3D-confined bands. Using our novel systematic confinement identification method from Refs. [36,61], we discover that there are in total 10 3D-confined bands for the same physical conditions. Figure 12 shows the confinement map of c = 3point-confined bands in an inverse woodpile superlattice with larger regular pore radii R = 0.27a, while varying the radius R' of the defect pores. The behavior of the bands is similar to that for R = 0.24a in Fig. 11, with groups of bands moving from the low-frequency edge of the band gap upwards and disappearing at the upper edge as R'/R increases. There are, however, three qualitative differences compared to the R =0.24a case. First, in this case, c = 3 defect bands are observed



FIG. 13. Confinement map of point-confined c = 3 bands in an inverse woodpile superlattice with regular pore radius R = 0.18a and varying radius R' of the crossing defect pores. The case of the unperturbed crystal corresponds to R'/R = 1 and is denoted by the dashed vertical line. Each point represents the average reduced frequency of a point-confined band and the dashed red lines represent the edges of the band gap of an unperturbed crystal. The color and shape of the symbols correspond to their values of maximum energy density Ω , as described in the legend.

already for R' = 1.1R, thus reducing the pore radius threshold compared to R = 0.24a. Second, the bands with high-energy concentration $\Omega > 10$ are now sprinkled across the whole plot, suggesting that energy concentration prefers larger pore radii R.

Third, we see here several bands exceeding the top of the band gap for R' < R, which cannot be explained by the differences in silicon volume fraction. These bands are indeed 3D-confined, as confirmed by visually inspecting their energy density distribution, so this is not an artifact of the employed method. This observation confirms what was already hinted at by the results of Ref. [61], namely that the confinement does not suddenly stop at the top edge of the band gap, for R' < R. At frequencies above the point-confined c = 3 bands, linearly confined c = 2 bands appear, as seen in Ref. [61]. It follows from this observation that the bands at the top of the band gap lose their confinement properties only gradually, transitioning from c = 3 through c = 2 until they become extended c = 0bands. Such (partially) confined bands outside the band gap may possibly correspond to symmetry-protected bound states in the continuum; see Ref. [70]. In contrast, the lower band gap edge appears to be a much stricter boundary, even when the slight shift with respect to the change in the silicon volume fraction is accounted for. This has also been observed in experiments, where the position of this edge provided great help when analyzing the wave confinement and connecting the experiments with the theory [37]. Analogously, for R' > Rthe role of the band edges is exchanged and the upper band edge acts as a hard boundary, only slightly shifted by the change in the silicon volume fraction, while at the lower band edge the bands seem to lose their confinement properties only gradually.

Figure 13 shows the map of c = 3 point-confined bands in an inverse woodpile superlattice with small regular pores of



FIG. 14. Confinement map of point-confined c = 3 bands in an inverse woodpile superlattice with varying regular crystal pore radii R and constant ratio R'/R = 0.5. Each data point represents the average reduced frequency of a point-confined band and the dashed red lines represent the edges of the band gap of an unperturbed crystal. The color and shape of the symbols correspond to their maximum energy densities Ω , as given in the legend.

the radius R = 0.18a, while varying the radius R' of the defect pore. Once again, we observe groups of bands emerging from the top of the band gap and descending into the gap with decreasing pore radius. A crucial observation here is that no 3D-confined bands have been found for the defect pore radii R' > 0.6R, including no confined acceptorlike bands for R' > R. Notably, there is also a lack of bands with $\Omega > 10$, which means that for R = 0.18a the energy concentration is in general weaker than in the case of larger pores.

There seems to be a significant preference for both the existence and the strength of 3D confinement in structures with larger regular pores. This discovery is of considerable practical importance, since in photonic crystal fabrication it is easier to fabricate high-quality pores when they have smaller radii [54], as larger pores increase the likelihood that the structure collapses. (For examples of some successfully fabricated and studied structures as well as a collapsed one, see Refs. [59,71].) Our research thus offers important guidelines for manufacturing inverse woodpile superlattices for confinement experiments and applications.

B. Confinement versus regular pore radius

Figure 14 shows the map of c = 3 point-confined bands in an inverse woodpile superlattice from an alternative point of view, where the ratio between the defect and the regular pore radius R'/R = 0.5 is kept constant, whereas the radius of the crystal pores *R* is tuned. For viewing convenience, we also replotted these data in Fig. 15, where we subtract the band gap center frequency ω_c at each *R* from the band frequencies.

First of all, it is remarkable that even though the band gap has nonzero width, there are no 3D-confined bands for crystal pore radii R = 0.15a and 0.16a. This is not the case at the opposite side of the band gap, where 3D-confined bands appear even very close to its closing at R = 0.29a. Similarly to the other studied cases, we observe that high-energy



FIG. 15. Confinement map of point-confined c = 3 bands in an inverse woodpile superlattice with varying regular pore radius *R* and constant ratio R'/R = 0.5. This plot shows the same data as Fig. 14, but the frequency of each structure has been adjusted by subtracting the center of the band gap for each regular pore radius *R*. Each point represents the average relative frequency of a point-confined band and the dashed red lines represent the edges of the band gap of an unperturbed crystal. The color and shape of the symbols correspond to their values of maximum energy density Ω , as described in the legend.

densities $\Omega > 10$ appear only in structures with larger pore radii $R \ge 0.20a$. All these observations together agree with our statement above that the strongly confined bands are more abundant in structures with larger pores. There is also a visible movement of the confined bands from the top of the band gap towards its bottom, as R/a increases. These bands again form groups, which get more separated in frequency from each other as the band gap becomes wider.

VII. CONCLUSIONS

In this paper, we have performed a computational study of optical waves confined in 3D inverse woodpile photonic band gap cavity superlattices, with respect to the main structural parameters of the superlattices, namely the regular and the defect pore radii. We have created maps of 3D-confined bands via various cross-sections through the parameter space of the two pore radii, and we used these maps to analyze the influence of the superlattice structure on the confinement. We find that larger regular pore radii favor more confined bands, and these bands also tend to have higher concentrated energy densities. Simultaneously, we have analyzed the symmetries of salient 3D-confined bands in 3D inverse woodpile photonic band gap cavity superlattices. We conclude that the photonic band gap cavity superlattice bands exhibit very different symmetries compared to electronic orbitals known from solidstate physics, which is caused by the underlying crystal geometry and facilitated by the fact that our states here derive from global Bloch states, whereas atomic orbitals are localized. We propose that attention should be given to band symmetries in "photonic solid-state matter" and their influence on the properties of these materials.

We have analyzed the potential of the inverse woodpile photonic band gap cavity superlattices for cavity QED applications. To this end, a large concentration of energy density, proportional to LDOS, must be present in the defect-pore region. We find that even though the acceptorlike structures with defect pores larger than the regular pores may offer higher energy concentration, this energy is mostly concentrated in small regions of silicon and decays rapidly in air. On the other hand, the investigated donorlike structure, despite exhibiting less concentrated energy density, provides overall higher values of energy density within the cavity due to larger silicon and smaller air volumes inside. Therefore, donorlike structures seem to be more favorable for spontaneous emission control.

In future, more data should be gathered and analyzed to obtain an even deeper understanding of the confinement behavior of inverse woodpile superlattices. Analyzing electric field components instead of only the energy density will provide further insight into the mode topology of each band, especially regarding even/odd symmetries. Moreover, a future study should be extended to encompass not only 3D-confined bands but also 2D-confined ones, which have been previously shown to exist in these structures as well. Finally, this type of investigation should be extended to other classes of photonic superlattices that are being pursued in other labs worldwide.

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