

Variational analysis for photonic molecules: Application to photonic benzene waveguides

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(Received 21 April 2003; published 23 September 2003)

A type of artificial molecule, called the photonic molecule, is investigated. It consists of coupled-defect atoms in photonic crystals. We theoretically present a method to determine the frequency of each resonant mode for the photonic molecule. Within the major band gap, the photonic molecule confines the resonant modes that are closely analogous to the ground-state molecular orbitals of an analogous chemical molecule and the corresponding electromagnetic spectrum is also isomorphous to the electric energy levels. By employing the variational theory, the constraint determining the resonant coupling is formulated, which is consistent with the results of both the scattering matrix method and the group analysis. In addition, a type of photonic waveguide is proposed for the two-dimensional system that manipulates the mechanism of photon hopping between photonic benzene and offers an optical feature of twin waveguiding bandwidths.

DOI: 10.1103/PhysRevE.68.036611

PACS number(s): 42.82.Et, 42.70.Qs, 42.60.Da, 71.15.Ap

I. INTRODUCTION

In the past decade, photonic defects have attracted much attention because of their scientific and technological applications in the realization of high-Q microcavities or high transmission waveguides (WGs) [1–7]. A defect atom can be embedded in a photonic crystal by perturbing the dielectricity of a selected crystal “atom” that has photons with certain frequencies locally trapped within the band gap of the surrounding crystal structure. If defect atoms are embedded by design to form the so-called line defect then, within the band gap, it may provide a mechanism of photon propagation via hopping from one defect atom to its neighbors with a high transmission [8–11]. Consequently, the integrated optical circuits of functional elements can be realized through skillful integration of photonic defects and WGs, and is expected to offer potential applications in telecommunication [12,13].

An important point that has received little attention is that the formation of photonic WGs is conventionally considered as the arrangement of the desired defect atoms along a line, however, this approach has limited the potential of development. We suggest a broader vision of the manipulation of defect atoms through the investigation of photonic molecules, which are defined as follows. In photonic crystals, the defect atoms are closely arranged to form a structure that is similar to a real molecule—so named because, within the major band gap, the resonant modes confined by such a structure are closely analogous to the ground states of the molecular orbitals (MOs) of a real molecule. For example, Fig. 1(a) shows a two-dimensional (2D) photonic molecule named as the photonic benzene, whose defect modes are shown in Fig. 3. By employing the variational theory, the constraint determining the resonant coupling of photonic molecule is formulated, which is consistent with the results from those of both the scattering solution and the group analysis. In particular, manipulating the mechanism of photon hopping between photonic benzenes can provide the function of guiding photons along the benzene chain with a

very high transmission, and presents an optical feature of twin waveguiding bandwidths in the 2D system, as shown in Fig. 4.

Sievenpiper and co-workers are the first to propose the concept of embedding photonic defects in a photonic crystal by following the geometry of chemical molecules [14]. They have experimentally demonstrated that the frequency level structures of four photonic molecules correspond to the energy levels of the corresponding molecules in chemistry. Nevertheless, the theoretical investigation on coupled-defect modes of the photonic molecule is necessary for further application of photonic waveguides. In this study, we apply a variational approach to calculate the various coupled-defect modes for photonic molecules, and for the 2D system we further manipulate the four modes that are found in photonic benzene to constitute the so-called benzene waveguides.

II. THE VARIATIONAL METHOD

Because of the importance of interpreting the mechanism of defect coupling, there are mainly two solid-state theoretical approaches, the tight-binding (TB) [8,9,11,15] and the Wannier function methods [16–18], which have been applied to study the coupled cavities. The photonic version of TB method extends the idea of linear combination of atomic orbitals (LCAO), in which the defect modes are analogous to the atomic wave function, and suppose that only the nearest-neighbor couplings are relevant to find the dispersion relation for waveguide mode. For the latter, the localized defect modes are expanded by Wannier functions to calculate their intensity variations, where the Wannier functions are calculated by plane-wave method or TB method coupled with supercell approximation. Here, another powerful approach of variational analysis is proposed for many defect-atoms system.

Considering first an electric resonant mode $\mathbf{E}_d(\mathbf{r})$ of a single defect in a finite-size photonic crystal, the Maxwell equations obeyed by $\mathbf{E}_d(\mathbf{r})$ can be further simplified as

$$\hat{\mathbf{H}}\mathbf{E}_d(\mathbf{r}) = \epsilon_d(\mathbf{r})(\omega_d/c)^2\mathbf{E}_d(\mathbf{r}), \quad (1)$$

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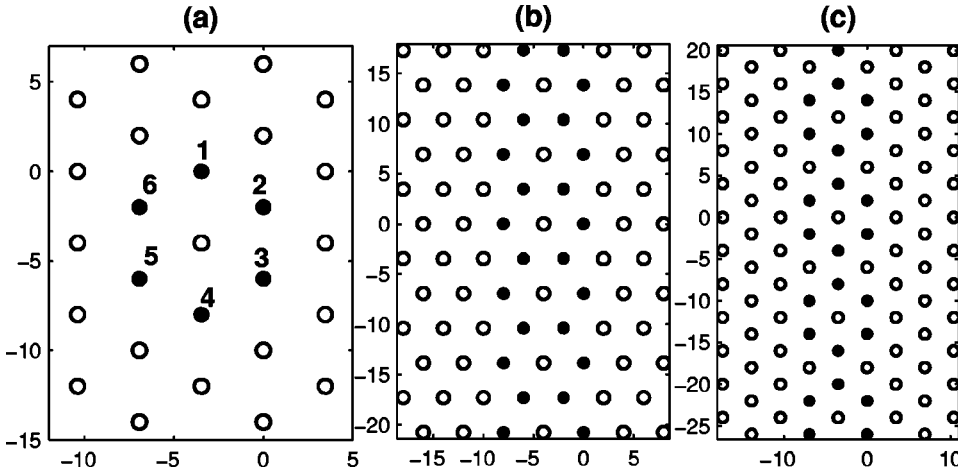


FIG. 1. Formation of (a) photonic benzene, (b) benzene WG of π type, and (c) benzene WG of σ type in a 2D hexagonal crystal; each solid dot denotes a defect atom of radius ρ .

where the operator $\hat{\mathbf{H}}$ is defined as $-\nabla^2$ for the TM modes of the 2D system or $\nabla \times \nabla \times$ for the 3D system. Also, $\epsilon_d(\mathbf{r})$ denotes the dielectric constant of the single-defect system and ω_d is the eigenfrequency of the eigenmode $\mathbf{E}_d(\mathbf{r})$. Those modes that occur within the major band gap are of maximum concern in this paper and can be taken as real and normalized by

$$\langle \mathbf{E}_d(\mathbf{r}) | \epsilon_d(\mathbf{r}) | \mathbf{E}_d(\mathbf{r}) \rangle \stackrel{\text{def}}{=} \int_{\text{domain}} \epsilon_d(\mathbf{r}) \mathbf{E}_d(\mathbf{r}) \cdot \mathbf{E}_d(\mathbf{r}) d\mathbf{r} = 1.$$

For the same photonic crystal considered in Eq. (1) but embedded with a photonic molecule, the allowed resonant modes are assumed as a superposition of the individual defect mode. Basically, it is analogous to the idea of LCAO, namely,

$$\mathbf{E}_n(\mathbf{r}) = \sum_{i=1}^{n_d} C_{ni} \mathbf{E}_d(\mathbf{r} - \mathbf{R}_i), \quad (2)$$

where $\mathbf{E}_n(\mathbf{r})$ is the n th resonant mode of the photonic molecule, n_d the number of defect atoms, C_{ni} the undetermined coefficient, and \mathbf{R}_i the coordinates of the i th defect atom. Similarly, $\mathbf{E}_n(\mathbf{r})$ satisfies Eq. (1) but with $\epsilon_d(\mathbf{r})$ replaced by the dielectric constant $\epsilon_{pm}(\mathbf{r})$ of the photonic molecule system and ω_d replaced by the frequency ω_n of the eigenmode $\mathbf{E}_n(\mathbf{r})$, that is,

$$\hat{\mathbf{H}} \mathbf{E}_n(\mathbf{r}) = \epsilon_{pm}(\mathbf{r}) (\omega_n/c)^2 \mathbf{E}_n(\mathbf{r}). \quad (3)$$

Equation (2) associated with Eq. (3) is a linear variational problem. Assigning different coefficient C_{ni} to each mode \mathbf{E}_d may create different \mathbf{E}_n , but the structure of photonic molecule will determine which resonant modes are allowed. This inference will be reflected on restricting C_{ni} to satisfy the minimum of functional frequency, defined as

$$\Omega(C_{ni}) \stackrel{\text{def}}{=} \frac{\langle \mathbf{E}_n(\mathbf{r}) | \hat{\mathbf{H}} | \mathbf{E}_n(\mathbf{r}) \rangle}{\langle \mathbf{E}_n(\mathbf{r}) | \epsilon_{pm}(\mathbf{r}) | \mathbf{E}_n(\mathbf{r}) \rangle} = \frac{\sum_{ij} C_{ni} C_{nj} \mathbf{H}_{ij}}{\sum_{ij} C_{ni} C_{nj} \mathbf{S}_{ij}}.$$

Namely, Ω is equivalent to the familiar Rayleigh-Ritz principle. Here \mathbf{H}_{ij} and \mathbf{S}_{ij} denote, respectively, the elements of the Hamiltonian matrix and the overlap matrix. According to Eqs. (1) and (2), \mathbf{H}_{ij} can be written as

$$\mathbf{H}_{ij} = \langle \mathbf{E}_d(\mathbf{r} - \mathbf{R}_i) | \hat{\mathbf{H}} | \mathbf{E}_d(\mathbf{r} - \mathbf{R}_j) \rangle = \begin{cases} (\omega_d/c)^2 = \alpha & \text{for } i=j \\ (\omega_d/c)^2 \beta_1 & \text{for } (i,j) \text{ being the nearest-neighbor} \\ (\omega_d/c)^2 \beta_2 & \text{for } (i,j) \text{ being the second-neighbor} \\ (\omega_d/c)^2 \beta_3 & \text{for } (i,j) \text{ being the third-neighbor,} \end{cases}$$

where $\beta_{(ij)} = \langle \mathbf{E}_d(\mathbf{r} - \mathbf{R}_i) | \epsilon_d(\mathbf{r} - \mathbf{R}_j) | \mathbf{E}_d(\mathbf{r} - \mathbf{R}_j) \rangle$ denotes the hopping integral whose magnitude measures the coupling strength and decays rapidly with increasing the distance $|\mathbf{R}_i - \mathbf{R}_j|$, i.e., $|\beta_1| > |\beta_2| > |\beta_3|$ (the more the defect sites split, the weaker their coupling [19]). Therefore, hopping terms

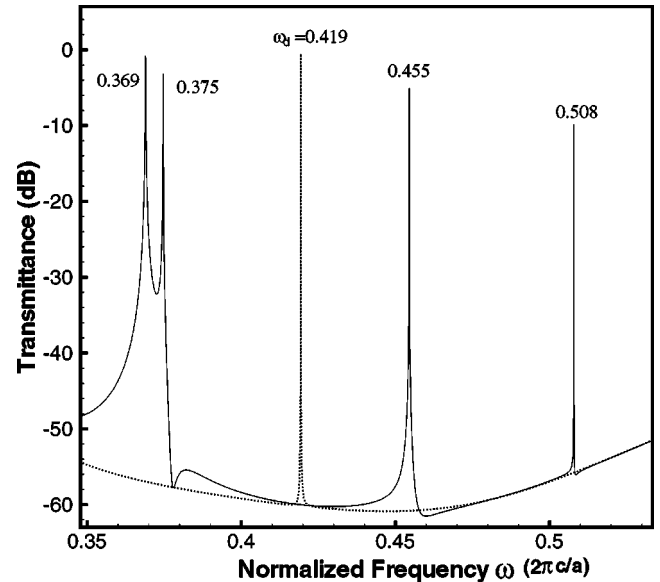


FIG. 2. Transmittance amplitude of electric field as a function of normalized frequency for a 2D photonic benzene (solid curve) and a defect atom (dotted curve). The marked values are four frequencies of the high- Q modes which are split from the ω_d due to defect coupling and fall in the major band gap whose range is as shown in Fig. 4.

TABLE I. The calculated values of normalized resonant frequencies and hopping parameters for photonic benzene with different ρ but the same dielectric constant as the host cylinders.

ρ	ω_d	ω_1	ω_2	ω_3	ω_4	β_1	β_2	β_3
0.0	0.419	0.455	0.375	0.369	0.508	0.178	0.051	-0.010
0.05	0.417	0.452	0.373	0.367	0.505	0.177	0.051	-0.009
0.1	0.409	0.442	0.369	0.361	0.493	0.171	0.048	-0.006
0.15	0.395	0.423	0.361	0.351	0.468	0.155	0.040	-0.002

can be classified according to the separation of the coupled defects. Here, only three relevant hopping terms are considered. Moreover, under the assumption that each individual defect mode is highly localized around its defect site, the field overlap between different defect atoms is small and the overlap integral \mathbf{S}_{ij} can thus be approximated as

$$\mathbf{S}_{ij} = \langle \mathbf{E}_d(\mathbf{r} - \mathbf{R}_i) | \epsilon_{pm}(\mathbf{r}) | \mathbf{E}_d(\mathbf{r} - \mathbf{R}_j) \rangle \approx \delta_{ij}. \quad (4)$$

Now, vary C_{ni} to minimize the functional frequency Ω , with the necessary condition of $\partial\Omega/\partial C_{ni} = 0$, $i = 1, 2, \dots, n_d$. One can obtain

$$\sum_{j=1}^{n_d} [\mathbf{H}_{ij} - (\omega_n/c)^2 \delta_{ij}] C_{nj} = 0.$$

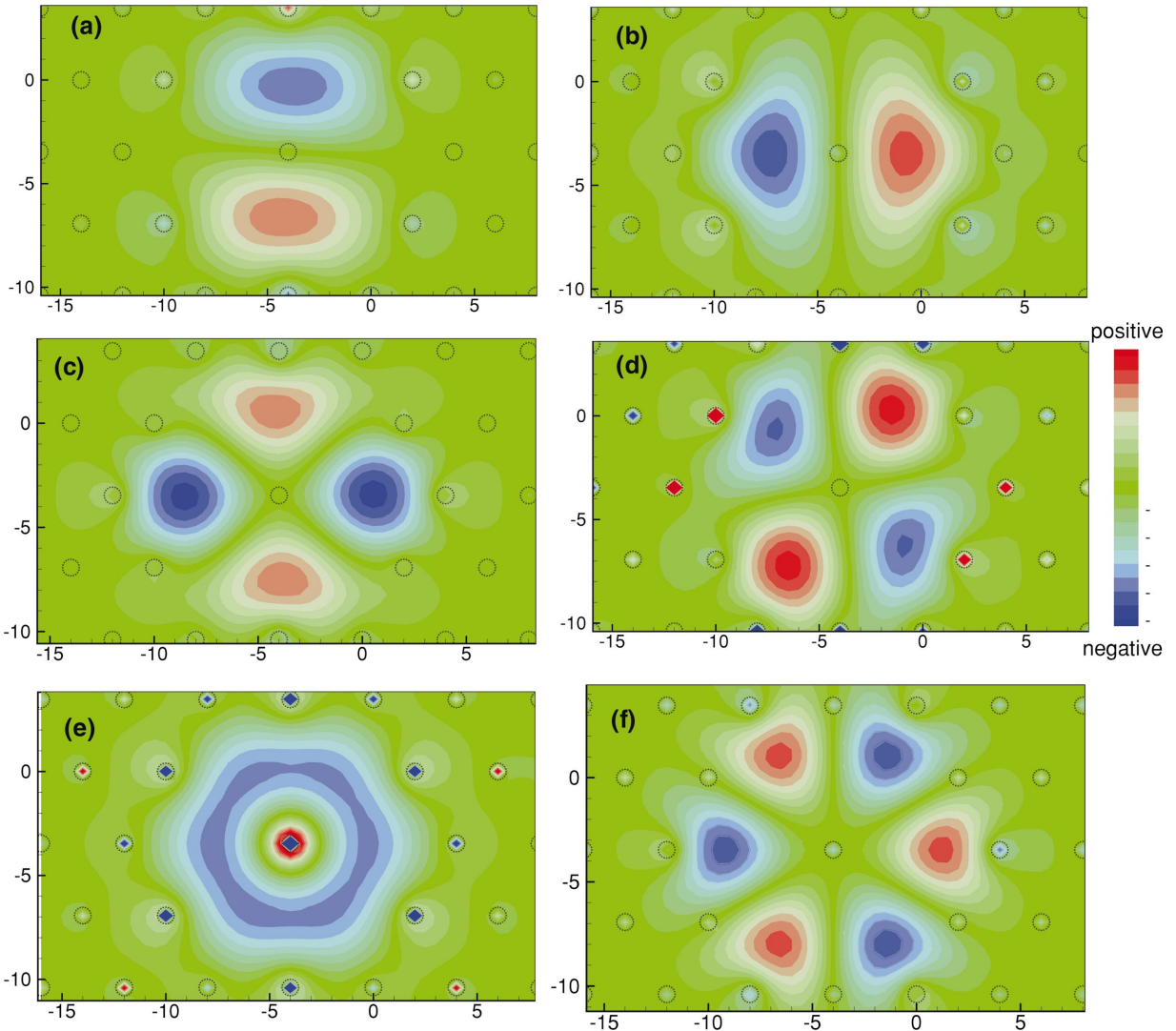


FIG. 3. (Color) Resonant electric field pattern in a 2D photonic benzene of $\rho=0$ for the six lowest resonant modes with normalized frequencies of (a) and (b) 0.369 with E_1 mode, (c) and (d) 0.455 with E_2 mode, (e) 0.375 with A_1 mode, and (f) 0.508 with B_2 mode. In general, the more the number of nodes, the higher the frequency.

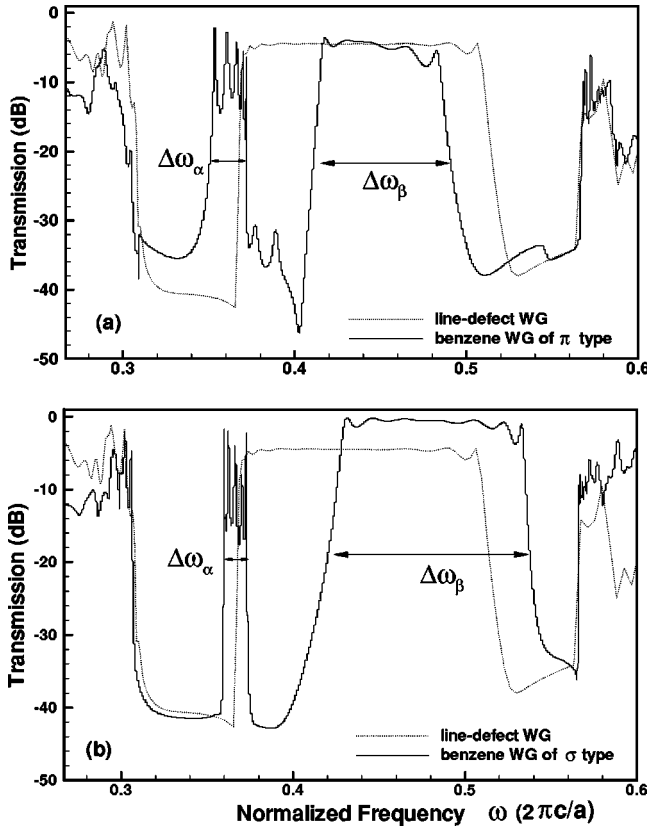


FIG. 4. Transmission created by the 2D benzene WGs of (a) π type and (b) σ type with $\rho=0.0$. Both types present the feature of twin waveguiding bandwidths, marked as $\Delta\omega_\alpha$ and $\Delta\omega_\beta$.

The constraint of resonant frequencies can thus be derived from the solvability condition of C_{ni} . This leads to

$$\det[\mathbf{H}_{ij} - (\omega_n/c)^2 \delta_{ij}] = 0. \quad (5)$$

Equation (5) indicates that the allowed resonant frequencies in a given photonic molecule are dominated by hopping

integrals. Furthermore, these hopping terms are dependent upon the dielectric structure of the photonic molecule. Therefore, every resonant mode is characterized by photonic molecule and exhibits different optical transmittance.

III. RESULTS FOR A PHOTONIC BENZENE

To check the accuracy of Eq. (5), we first apply Eq. (5) to the photonic benzene, which yields

$$\begin{vmatrix} \alpha - \gamma & \tilde{\beta}_1 & \tilde{\beta}_2 & \tilde{\beta}_3 & \tilde{\beta}_2 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \alpha - \gamma & \tilde{\beta}_1 & \tilde{\beta}_2 & \tilde{\beta}_3 & \tilde{\beta}_2 \\ \tilde{\beta}_2 & \tilde{\beta}_1 & \alpha - \gamma & \tilde{\beta}_1 & \tilde{\beta}_2 & \tilde{\beta}_3 \\ \tilde{\beta}_3 & \tilde{\beta}_2 & \tilde{\beta}_1 & \alpha - \gamma & \tilde{\beta}_1 & \tilde{\beta}_2 \\ \tilde{\beta}_2 & \tilde{\beta}_3 & \tilde{\beta}_2 & \tilde{\beta}_1 & \alpha - \gamma & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\beta}_2 & \tilde{\beta}_3 & \tilde{\beta}_2 & \tilde{\beta}_1 & \alpha - \gamma \end{vmatrix} = 0, \quad (6)$$

where we let $\gamma = (\omega_n/c)^2$ and $\tilde{\beta}_i = (\omega_d/c)^2 \beta_i$ for simplification. The determinant in Eq. (6) is called the sixth-order circulant and is equivalent to

$$\prod_{n=1}^6 [(\alpha - \gamma) + e_n \tilde{\beta}_1 + e_n^2 \tilde{\beta}_2 + e_n^3 \tilde{\beta}_3 + e_n^4 \tilde{\beta}_2 + e_n^5 \tilde{\beta}_1] = 0,$$

where e_1, e_2, \dots, e_6 are the six roots of unity, i.e., $e_n = \exp(2\pi i n/6)$. Hence, for $n=1, \dots, 6$, the frequencies ω_n of the six resonant modes \mathbf{E}_n can be found as

$$\omega_n = \omega_d \sqrt{1 + 2 \cos \frac{2\pi n}{6} \beta_1 + 2 \cos \frac{2\pi n}{3} \beta_2 + (-1)^n \beta_3}. \quad (7)$$

Obviously, Eq. (7) indicates that there are two doubly degenerate frequencies with $n=1,5$ and $n=2,4$, and two nondegenerate frequencies with $n=3$ and $n=6$, thus, four

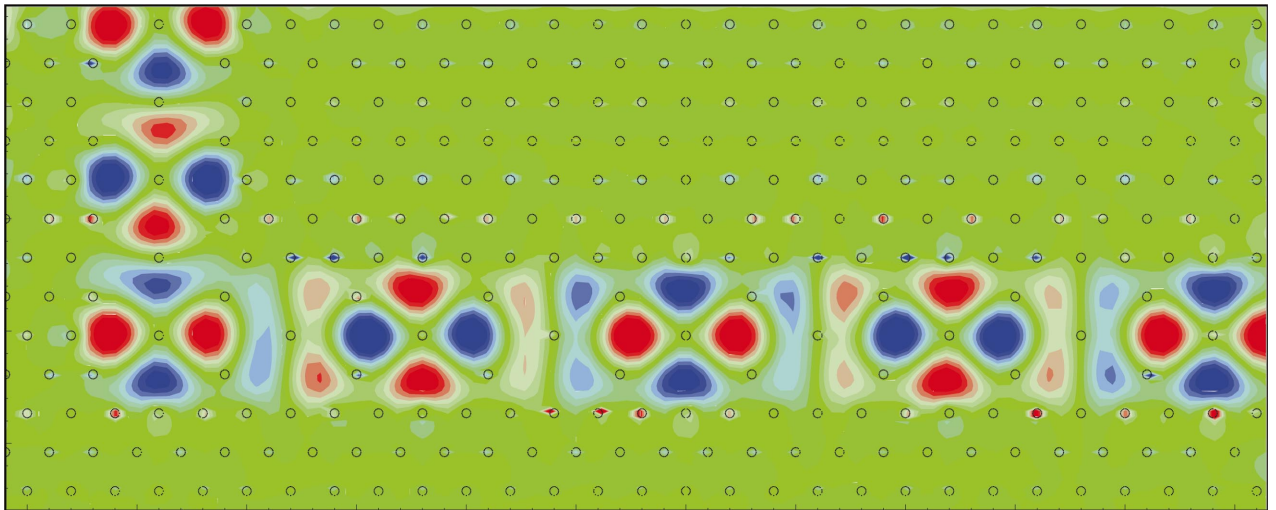


FIG. 5. (Color) Electric field distribution of a TM light with E_2 mode travels through a 90° bend in a 2D benzene WG where the junction connects a π -type WG with a σ type; incident wave with normalized frequencies 0.449 enters from the upper left.

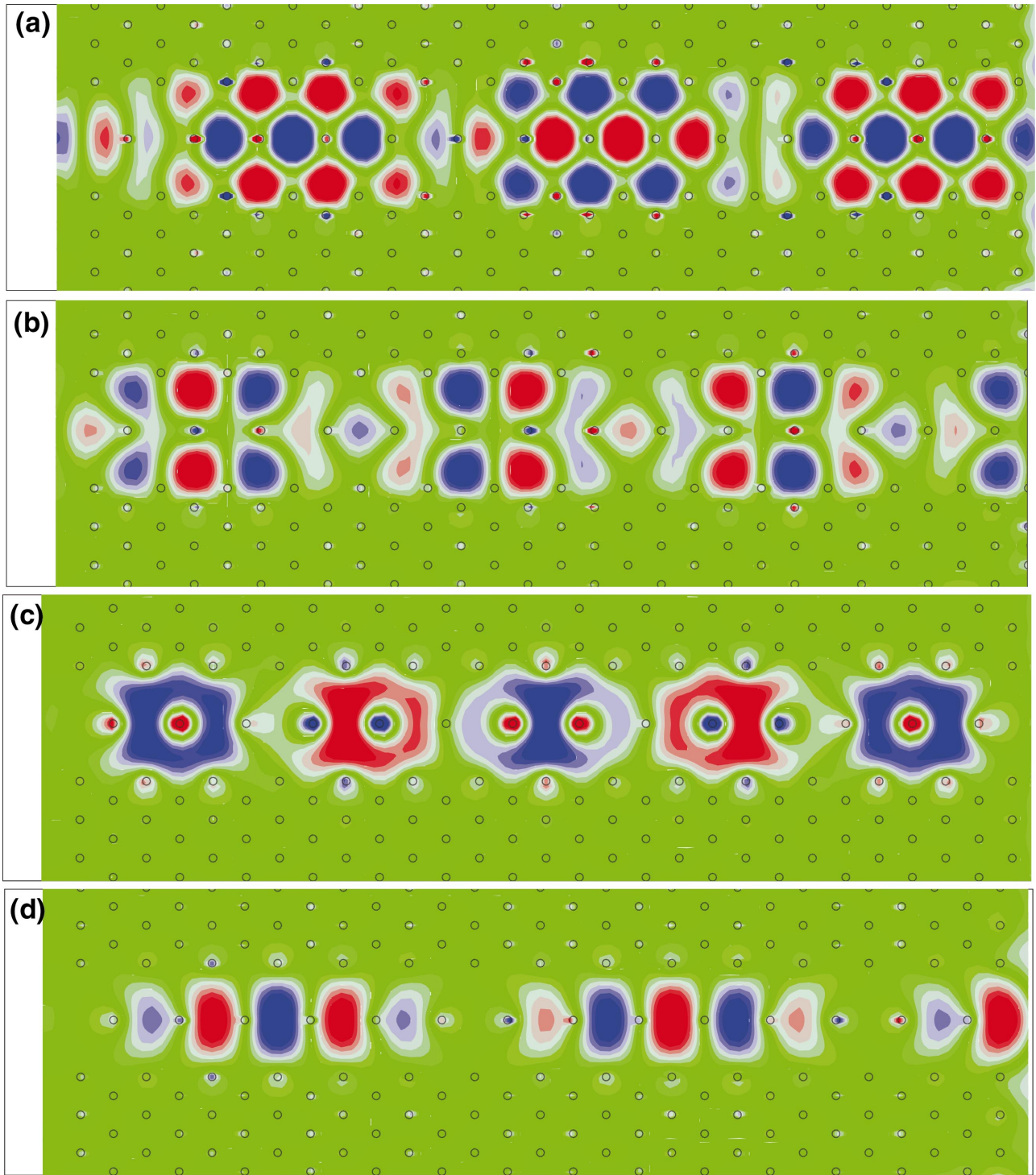


FIG. 6. (Color) Electric field distributions of a TM light with various modes travels (from right to left) through a 2D benzene WG of π type. The normalized frequencies from high to low are, respectively, (a) $\omega=0.480$ of E_2 mode, (b) $\omega=0.421$ of E_2 mode, (c) $\omega=0.370$ of A_1 mode, and (d) $\omega=0.354$ of E_1 mode.

high- Q resonant frequencies will occur within the major band gap. From the viewpoint of the symmetry group, the photonic benzene belongs to the point group C_{6v} for the 2D or D_{6h} for the 3D systems (cylinders with a finite height), whose irreducible representation Γ on defect sites can be reduced to the decomposition $\Gamma=A_1+B_2+E_1+E_2$ or $\Gamma=A_{2u}+B_{2g}+E_{1g}+E_{2u}$, respectively. Exactly speaking, it

again illustrates two doubly degenerate modes of E_1 (or E_{1g}) and E_2 (or E_{2u}), and two nondegenerate modes of A_1 (or A_{2u}) and B_2 (or B_{2g}). Furthermore, these predictions are also consistent with the numerical solution of Eq. (3) that is calculated by scattering method (cf. Ref. [19]). The resultant transmittance for the 2D case is plotted in Fig. 2, and the allowed resonant modes are shown in Fig. 3, where we con-

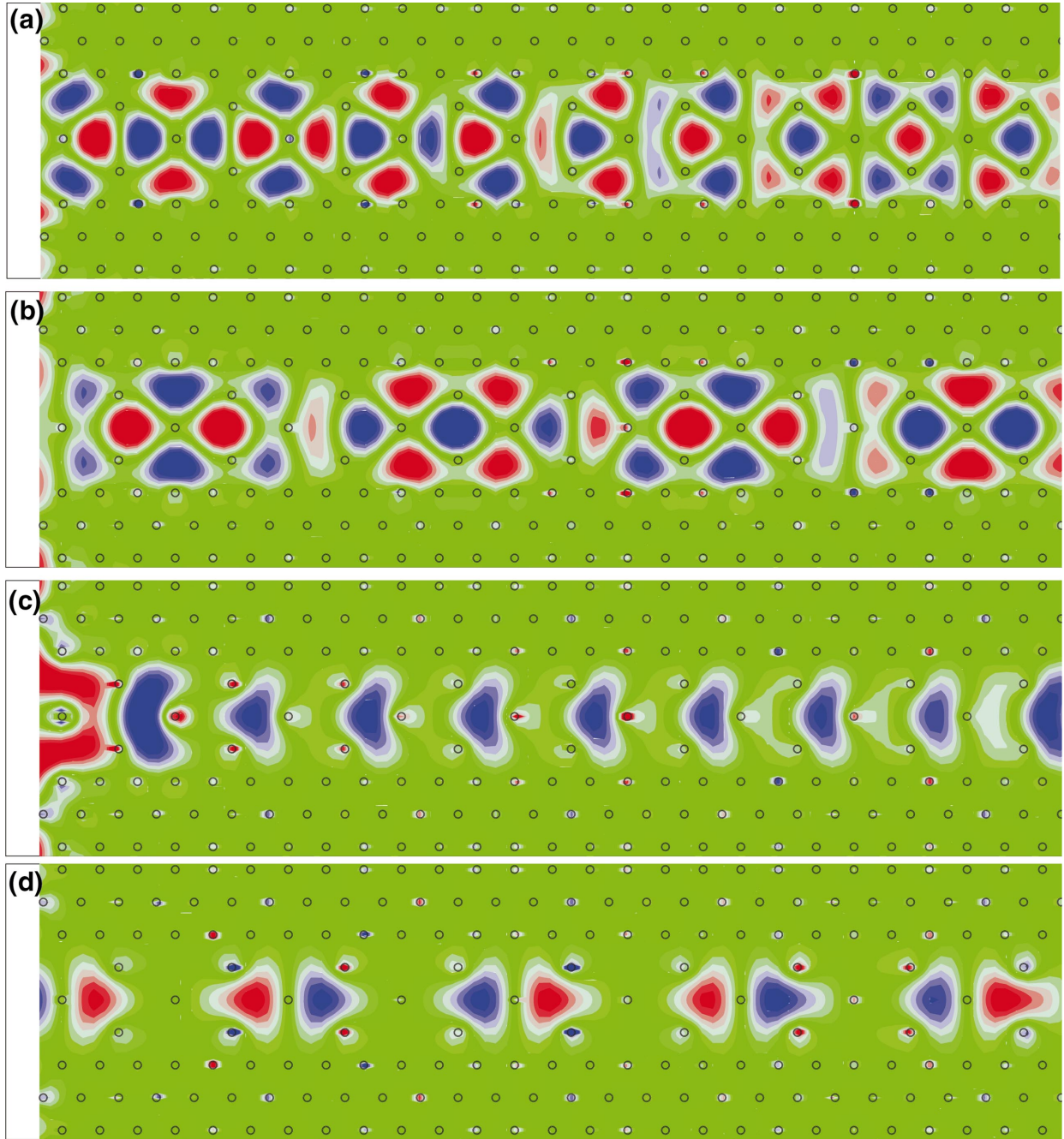


FIG. 7. (Color) Electric field distributions of a TM light with various modes travels (from left to right) through a 2D benzene WG of σ type. The normalized frequencies from high to low are, respectively, (a) $\omega=0.500$ of B_2 mode, (b) $\omega=0.444$ of E_2 mode, (c) $\omega=0.371$ of A_1 mode, and (d) $\omega=0.362$ of E_1 mode.

consider a 2D finite-size hexagonal photonic crystal with a dielectric contrast ratio 8.4/1.0 (rod/background) and a radius-to-spacing ratio 0.4/4.0. The defect radius ρ is taken as zero.

Figure 2 shows four normalized resonant frequencies 0.369, 0.375, 0.455, and 0.508 that split from $\omega_d=0.419$ due to the defect coupling in a photonic benzene. By substituting these five frequencies into Eq. (7), the hopping terms β_1 , β_2 , and β_3 can be calculated by least-squares method, and they are 0.178, 0.051, and -0.010 , respectively. Table I summarizes four cases of defect sizes whose dielectric constant is assumed to be the same as that of the host cylinders,

in which all the values of hopping parameters achieve the accuracy of two decimal places for Eq. (7). It clearly shows that the larger the defect radius is, the smaller hopping parameters. This means that the defect couplings in photonic benzene become weaker as the defect radius is increased. Moreover, when the defect radius ρ is increased up to about 0.2, the property of four transmittance peaks disappears because of which the shallow perturbation of dielectricity for defect atoms will create shallow modes [1].

In fact, Eq. (3) is equivalent to the effective Schrödinger equation of Hückel π -electron theory (developed in 1931

[20]) if we make the resonant modes of 3D photonic benzene to be analogous to the π electrons of benzene molecule. However, Eq. (3) is much simpler. Theoretically, the π electrons arise from a planar unsaturated organic molecule whose MOs can be divided into the σ and π MOs according to the reflection symmetry in the molecular plane. Both systems belong to the same point group D_{6h} and have the same degeneracy (cf. Ref. [21], p. 261), but possess completely different meanings. Conceptually, the photonic molecule acts as a perfect model of artificial molecule, since the resonant modes are much easier to be realized than the bonding orbitals of real molecule. Similar phenomena can also be found in the quantum-dot molecules [22] or the coupled pairs of GaAs cavities (note that these systems are also termed as photonic molecule, cf. Bayer *et al.* [23]). Figure 3 shows the lowest resonant modes allowed in a 2D photonic benzene with $\rho = 0.0$, and they are labeled according to the symmetry species of the group C_{6v} , which are analogous to the six π MOs of benzene molecule but lack the C_{1h} symmetry.

IV. APPLICATION TO PHOTONIC BENZENE WAVEGUIDES

In this section, we first apply the modular concept to photonic benzene to create the photonic WG and called these WGs as benzene WGs. In the chemical terminology, benzene WGs can be classified as π and σ types corresponding to the bonding types between two real benzene rings, as illustrated in Figs. 1(b) and 1(c), and their transmission spectrum are calculated by using the scattering matrix method [19]. The incident electromagnetic waves are considered to propagate from top to bottom of Figs. 1(b) and 1(c), and the measuring line is set at the bottom of each crystal. Note that the benzene WGs calculated in this section are all 2D systems.

It is remarkable that transmission of the benzene WGs reveals the special feature of twin waveguiding bandwidths marked as $\Delta\omega_\alpha$ and $\Delta\omega_\beta$, where $\Delta\omega_\alpha < \Delta\omega_\beta$, as shown in Fig. 4. This means that the benzene WGs are able to provide two working bandwidths at the same time. For these two types, the σ type of benzene WG is numerically proved to possess the wider waveguiding bandwidth and the higher transmission than π type. Actually, the second bandwidth of

π -type WG has upper bound at 0.48; it does not include the B_2 mode so that the B_2 mode is forbidden by π -type WGs.

Choosing the E_2 mode as an example, Fig. 5 shows that a TM light with the E_2 mode travels through a 90° bend from the π type to the σ type. Of course, the same phenomenon can also be observed in other modes. In addition, Figs. 6 and 7, respectively, show the propagation of various resonant modes in π -type and σ -type benzene WG, where the incident frequencies are considered from high to low with various modes. Each mode owns its waveguiding width that is separate from each other. Particularly, this feature has exceeded the traditional line-defect WG in the propagable modes.

V. CONCLUSION

In this study, we suggest a practicable idea for the manipulation of photonic defects, which includes the so-called photonic molecule and benzene WG. The optical properties of photonic molecules has been investigated by variational theory, which shows that the allowed resonant frequencies inside a photonic molecule are dominated by hopping parameters through the constraint (5). Taking the photonic benzene as an example, six resonant modes with two doubly degenerate and two nondegenerate modes are found and verified by both the scattering matrix method and the group theory. Especially, the benzene WGs created by the modular manipulation of photonic benzenes are demonstrated to possess the interesting feature of twin waveguiding bandwidths in the 2D system. Namely, benzene WGs provide two working bandwidths at the same time and make the function of guiding photons more flexible. Moreover, benzene WGs not only provide a high transmission, but also offer more modes for propagation.

ACKNOWLEDGMENTS

This work was supported by the *Global Fiberoptics, Inc.* I am grateful for useful discussions with Professor Yu-Li Lee (National Changhua University of Education), Professor Chii-Chang Chen, Professor Pi-Gang Luan (National Central University), Dr. Ya-Chih Tsai, and Dr. Zheng-Yao Su.

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