

# Investigation and Modification of Coupling of Photonic Crystal Defects \*

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We investigate the coupling of photonic crystal (PC) defects by using coupled-mode theory. The PC molecules formed by the coupling of two identical PC atoms are the focus of our study. It is revealed that the flatness of the transmission spectra of the PC molecules is determined uniquely by the phase shift of the travelling wave between the two coupled PC atoms. By properly adjusting the distance between the two constitutional PC atoms, we are able to modify the transmission spectrum of the resulting PC molecule. Theoretical analyses based on the coupled-mode theory are in good agreement with the simulation results obtained by the transfer matrix method and the finite-difference time-domain technique.

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Photonic crystals (PCs) formed by periodic modulation of dielectric constant or refractive index act as a promising platform to manipulate the flow of photons.<sup>[1]</sup> It has been recognized that photons can be strongly localized into a point defect in a similar way by which electrons are confined into an atom (or an impurity).<sup>[2]</sup> Due to this reason, a PC defect is sometimes referred to as a PC atom. Naturally, a structure consisting of two coupled PC defects is generally termed as a PC molecule. Indeed, there exist many similarities between the coupling of real or artificial atoms and that of PC atoms.<sup>[3-6]</sup>

When two identical atoms are brought together to form a molecule, one can expect the splitting of the Lorentz lineshape of the atom into two peaks that represent the so-called bonding and anti-bonding states.<sup>[4,5]</sup> The situation is very similar when two PC atoms are coupled to form a PC molecule.<sup>[4,5]</sup> Of course, there are some differences, for example, it has been found by one of the authors (S. Lan) that a broad and flat-on-top transmission spectrum may be formed for a PC molecule instead of the generation of bonding and anti-bonding states.<sup>[6]</sup> Coupled cavity waveguides (CCWs) can possess quasiflat impurity bands if the spectra of the corresponding PC molecules are flat on top.<sup>[7]</sup> Such quasiflat impurity bands are highly desirable for the construction of ultrafast all-optical devices because of their capability in effectively transmitting ultrashort pulses. Unfortunately, only a few PC molecules are found to possess flat transmission spectra and it severely limits the choices and flexibilities in designing PC-based devices.<sup>[6,7]</sup> Therefore, whether or not the coupling of PC atoms can be modified or engineered has become a great challenge.

It has been recognized that the coupling of PC atoms originates from the evanescent tunnelling of

the electromagnetic (EM) wave from one PC atom to another. Based on this, we can establish a physical model to describe the coupling of two PC atoms as schematically shown in Fig. 1. According to coupled-mode theory (CMT),<sup>[8]</sup> which has been widely used as an efficient tool in recent study of PCs,<sup>[9-12]</sup> the equations that describe the time variations of the energy amplitudes in the two coupled PC atoms are given by

$$\frac{dA}{dt} = \left( j\omega_{01} - \frac{1}{\tau_A} - \frac{1}{\tau_1} - \frac{1}{\tau_2} \right) A + \sqrt{\frac{2}{\tau_1}} s_{+1} + \sqrt{\frac{2}{\tau_2}} s_{+2}, \quad (1a)$$

$$s_{-1} = -s_{+1} + \sqrt{\frac{2}{\tau_1}} A, \quad s_{-2} = -s_{+2} + \sqrt{\frac{2}{\tau_2}} A, \quad (1b)$$

$$\frac{dB}{dt} = \left( j\omega_{02} - \frac{1}{\tau_B} - \frac{1}{\tau_3} - \frac{1}{\tau_4} \right) B + \sqrt{\frac{2}{\tau_3}} s_{+3} + \sqrt{\frac{2}{\tau_4}} s_{+4}, \quad (2a)$$

$$s_{-3} = -s_{+3} + \sqrt{\frac{2}{\tau_3}} B, \quad s_{-4} = -s_{+4} + \sqrt{\frac{2}{\tau_4}} B, \quad (2b)$$

where  $A$  and  $B$  represent the energy amplitudes in the two constitutional PC atoms;  $\omega_{10}$  and  $\omega_{20}$  are the resonant frequencies of the two PC atoms;  $1/\tau_A$  and  $1/\tau_B$  denote the internal decay rates of  $A$  and  $B$ ;  $1/\tau_1$  and  $1/\tau_2$  denote the external decay rates of  $A$  into port 1 and port 2; Similarly,  $1/\tau_3$  and  $1/\tau_4$  denote the external decay rates of  $B$  into port 3 and port 4;  $s_{+i}$  and  $s_{-i}$  ( $i = 1-4$ ) are the incoming and outgoing waves for the  $i$ th port, as shown in Fig. 1. Furthermore, the EM waves travelling along the internal channel between the two PC atoms satisfy

$$s_{+2} = \exp(-j\varphi) s_{-3}, \quad s_{+3} = \exp(-j\varphi) s_{-2}, \quad (3)$$

where  $\varphi$  represents the phase shift of an EM wave travelling from one PC atom to another. In the cases

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of  $\varphi \neq n\pi$  with  $n$  being an integer including zero, we obtain two coupled equations describing the PC molecule which can be written as

$$\frac{dA}{dt} = \left( j\omega_1 - \frac{1}{\tau_A} - \frac{1}{\tau_1} \right) A + \kappa_{AB} B + \sqrt{\frac{2}{\tau_1}} s_{+1}, \quad (4a)$$

$$\frac{dB}{dt} = \left( j\omega_2 - \frac{1}{\tau_B} - \frac{1}{\tau_4} \right) B + \kappa_{BA} A + \sqrt{\frac{2}{\tau_4}} s_{+4}, \quad (4b)$$

where

$$\omega_1 = \omega_{01} + \frac{1}{\tau_2 \tan \varphi}, \quad \omega_2 = \omega_{02} + \frac{1}{\tau_3 \tan \varphi}, \quad (5)$$

$$\kappa_{AB} = \kappa_{BA} = -\frac{j}{\sqrt{\tau_2 \tau_3} \sin \varphi}. \quad (6)$$

The transmission through the PC molecule is given by

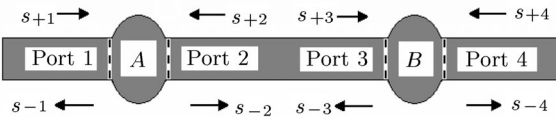
$$\begin{aligned} T &= \left| \frac{s_{-4}}{s_{+1}} \right|^2 \\ &= \left( \frac{4}{\tau'_1 \tau'_2 \tau'_3 \tau'_4 \sin^2 \varphi} \right) \cdot \left\{ \left[ \frac{1}{\tau'_1 \tau'_4} + \frac{1}{\tau_2 \tau_3 \sin^2 \varphi} \right. \right. \\ &\quad \left. \left. - \prod_{i=1}^2 (\omega - \omega_i) \right]^2 \right. \\ &\quad \left. + \left( \frac{\omega - \omega_1}{\tau'_4} + \frac{\omega - \omega_2}{\tau'_1} \right)^2 \right\}^{-1}, \quad (7) \end{aligned}$$

where  $\tau'_1 = (\tau_A^{-1} + \tau_1^{-1})^{-1}$ ,  $\tau'_4 = (\tau_B^{-1} + \tau_4^{-1})^{-1}$ . For a PC molecule formed by two identical and lossless PC atoms, we have  $\tau_{u1} = \tau_{u2} = \tau_{u3} = \tau_{u4} = \tau_u$ ,  $\omega_{01} = \omega_{02} = \omega_0$  and  $1/\tau_A = 1/\tau_B = 0$ . Also, it is noted that along the coupling direction the external decay rate can be related to the quality factor  $Q$  of the PC atoms, i.e.  $Q = \omega_0 \tau / 4$ . In this case, Eq. (7) can be written as

$$\begin{aligned} T &= \left[ T_0^{-1} - 8Q^2 \cos^2 \varphi \left( \frac{\omega}{\omega_0} - \frac{1}{4Q \tan \varphi} - 1 \right)^2 \right. \\ &\quad \left. + 64Q^4 \sin^2 \varphi \left( \frac{\omega}{\omega_0} - \frac{1}{4Q \tan \varphi} - 1 \right)^4 \right]^{-1}, \quad (8) \end{aligned}$$

where

$$T_0 = 4(2 + \sin^{-2} \varphi + \sin^2 \varphi)^{-1}. \quad (9)$$



**Fig. 1.** Schematic model describing the coupling of two PC atoms in a PC molecule based on the coupled-mode theory.

In the following discussion, it is temporarily assumed that the phase shift is insensitive to the frequency of the EM waves, at least in the narrow frequency range we considered. We will confirm later the

validity of this assumption by comparing the transmission spectra of PC molecules calculated by the CMT and those obtained by transfer matrix method (TMM)<sup>[13]</sup> and finite-difference time-domain (FDTD) simulation.<sup>[14]</sup>

According to Eq. (8), it is easy to deduce that the two peaks in the transmission spectrum which corresponds to the bonding and anti-bonding states appear at  $\omega = \omega_0$  and  $\omega = \omega_0[1 + (2Q \tan \varphi)^{-1}]$ . The transmission at the two peaks is unit. Also, it is important to note that the transmission at the valley between the two peaks is  $T_0$ . The corresponding frequency is  $\omega = \omega_0[1 + (4Q \tan \varphi)^{-1}]$ .

From Eq. (9), it is remarkable that the valley transmission  $T_0$  depends only on the phase shift  $\varphi$  and it has nothing to do with the other two parameters (i.e.  $\omega_0$  and  $Q$ ). Particularly, it is found that  $T_0$  is equal to the peak transmission (unit) as  $\varphi$  happens to be  $(n + 1/2)\pi$ , where  $n$  is an integer including zero. In this special case, Eq. (8) can be simplified as

$$T = [1 + 64Q^4(\omega/\omega_0 - 1)^4]^{-1}. \quad (10)$$

The spectrum in this case appears to be broad and flat-on-top as compared with the spectrum of the constitutional PC atoms. It can be attributed to the quartic item in the denominator of Eq. (10). In comparison, the corresponding item in the transmission spectrum of the PC atoms is only a square one.

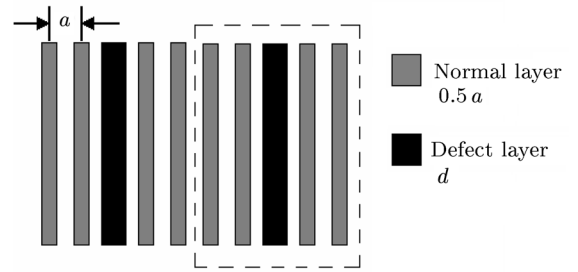
Based on the above discussion, we can conclude that the flatness of the transmission spectrum of a PC molecule is uniquely determined by a single quantity  $\varphi$ . From another point of view, we can extract the phase shift between the two coupled PC atoms from a single simulation. In addition, the difference in the spectral shape of different PC molecules can be interpreted as the difference in  $\varphi$ . Furthermore, this implies that we can modify the spectral shape through an adjustment of the phase shift and achieve flat spectra nearly for arbitrary PC atoms.

It is necessary to indicate that the case of  $\varphi = n\pi$  does not represent a coupling situation. By using the relations of  $s_{+2} = \pm s_{-3}$  and  $s_{+3} = \pm s_{-2}$  given by Eq. (3), the structure in this case can be considered as a single PC atom. Specifically,  $\varphi = 0$  means that there is no channel that connects the two PC atoms, implying that the two PC atoms are completely in coincidence with each other in space.

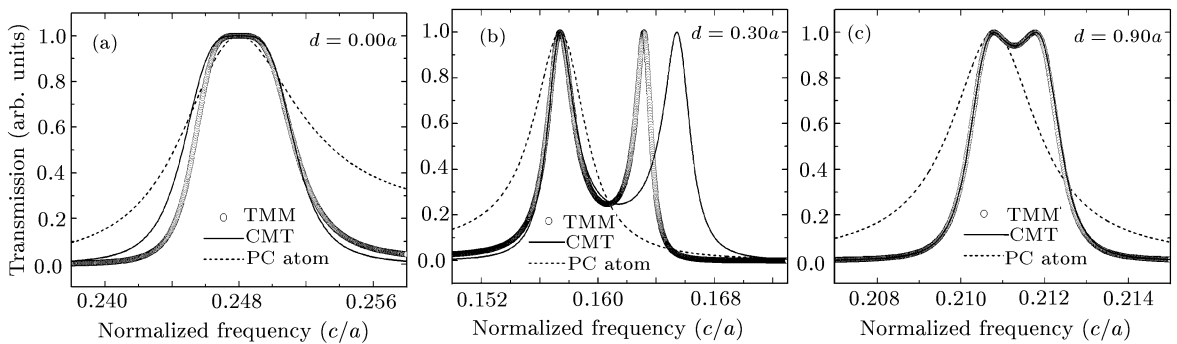
In order to verify the analyses presented above, let us first consider one-dimensional PC molecules. A typical case is shown in Fig. 2. The PC atom forming the PC molecule is indicated by a dashed box. It is derived from a PC consisting of five periodically placed dielectric layers with a refractive index of  $n_{\text{high}} = 3.4$  and a thickness of  $d_0 = 0.5a$ , where  $a$  is the lattice constant of the PC. The background is air ( $n_{\text{low}} = 1.0$ ). The PC atom is formed by modifying the thickness of

the central layer to a value of  $d$ . We have calculated the transmission spectra for PC molecules in which  $d = 0.00a$ ,  $0.30a$  and  $0.90a$  by TMM. The results are presented in Figs. 3(a), 3(b) and 3(c) by open circles. In all the cases, the transmission spectra of the constitutional PC atoms are also plotted by dashed curves for reference. According to the discussion in previous section, we can easily extract in each case the phase shift between the two PC atoms from the transmission at the valley of the spectrum of the resulting PC molecule. In Fig. 4, we plot the relationship between  $T_0$  and  $\varphi$  which is given by Eq. (9). It can be seen that  $T_0$  approaches the peak transmission (or unit) as  $\varphi$  drops in the region of  $(0.32 - 0.68)\pi$ . Out of this region, a sharp decrease in  $T_0$  occurs, leading to the formation of bonding and anti-bonding states. The

filled circles 1, 2 and 3 indicate the values of  $T_0$  and  $\varphi$  for the three PC molecules shown in Figs. 3(a), 3(b) and 3(c), respectively.



**Fig. 2.** Schematic of the one-dimensional PC molecule studied. The dashed box indicates one of the constitutional PC atoms.



**Fig. 3.** Comparison of the transmission spectra calculated by CMT and those simulated by TMM for three one-dimensional PC molecules: (a)  $d = 0.00a$ ; (b)  $d = 0.30a$ ; (c)  $d = 0.90a$ .

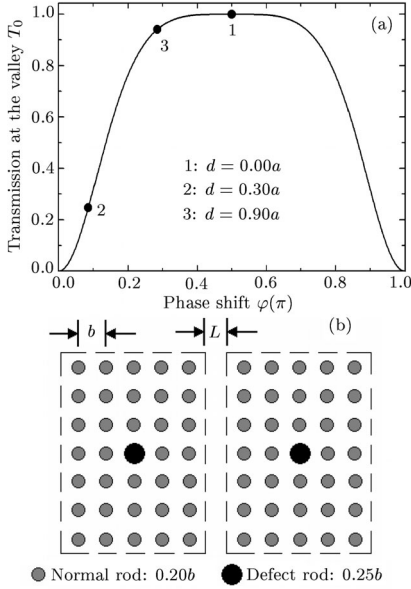
In order to verify the results deduced by CMT, we have calculated the transmission spectra of the three PC molecules by substituting the phase shift extracted above and the resonant frequency and  $Q$  factor extracted from the PC atom into Eq. (8). They are also presented in Figs. 3(a), 3(b) and 3(c) by solid curves. Obviously, very good agreement is achieved between the calculated results by CMT and the simulated results by TMM for the PC molecules of  $d = 0.00a$  and  $d = 0.90a$ . It indicates that the physical model based on CMT is valid for the description of the coupling of PC atoms. In addition, it is confirmed that the transmission spectrum of a PC molecule is uniquely determined by the phase shift which is nearly independent of frequency in the frequency range of the spectrum. As for the PC molecule of  $d = 0.30a$ , a discrepancy is found for the high-frequency peak. In our case, the first band gap for the PC ranges from  $0.150c/a$  to  $0.270c/a$ , where  $c$  is the speed of light in vacuum. The defect mode for the PC atom of  $d = 0.30a$  is very close to the edge of the dielectric band ( $\omega_0 = 0.157c/a$ ). Thus, it is thought that the coupling of this defect mode with the guided modes in the dielectric band is responsible for the discrepancy we observed.

It has been clarified that the flatness of the trans-

mission spectra of PC molecules is governed uniquely by the phase shift between the two coupled PC atoms. Therefore, we can control or modify the transmission spectra of PC molecules by adjusting the phase shift. A simple way to adjust the phase shift between the two PC atoms is to displace one PC atom from another along the coupling direction by a distance  $L$ . Here, we use a two-dimensional PC atom to demonstrate that we can tailor the transmission spectra of PC molecules. The two-dimensional PC atom (indicated by a dashed box) and molecule are schematically shown in Fig. 4(b). The PC is composed of a square lattice of dielectric rods with a refractive index of  $n_{\text{high}} = 3.4$  embedded in air ( $n_{\text{low}} = 1.0$ ). The radius of the dielectric rods  $r_0$  equals  $0.20b$ , where  $b$  is the lattice constant of the PC. The PC defect is introduced by changing the radius of the central rod in the PC atom to a value of  $r$ . The first band gap for the transverse magnetic polarization extends from  $0.289c/b$  to  $0.420c/b$ .  $L$  can be a positive or negative value or zero. Thus, the phase shift between the two PC atoms now becomes  $\varphi = \varphi_0 + 2\pi L/\lambda_0$ , where  $\varphi_0$  is the phase shift between the two PC atoms without any displacement ( $L = 0$ ) and  $\lambda_0$  is the resonant wavelength of the PC atom in air. Thus, we can modify the

phase shift without changing the other two parameters included in Eq. (8), i.e.  $\omega_0$  and  $Q$ .

We have employed a FDTD simulation to calculate the transmission spectra of the PC molecules formed by two identical PC atoms ( $r = 0.25b$ ) with



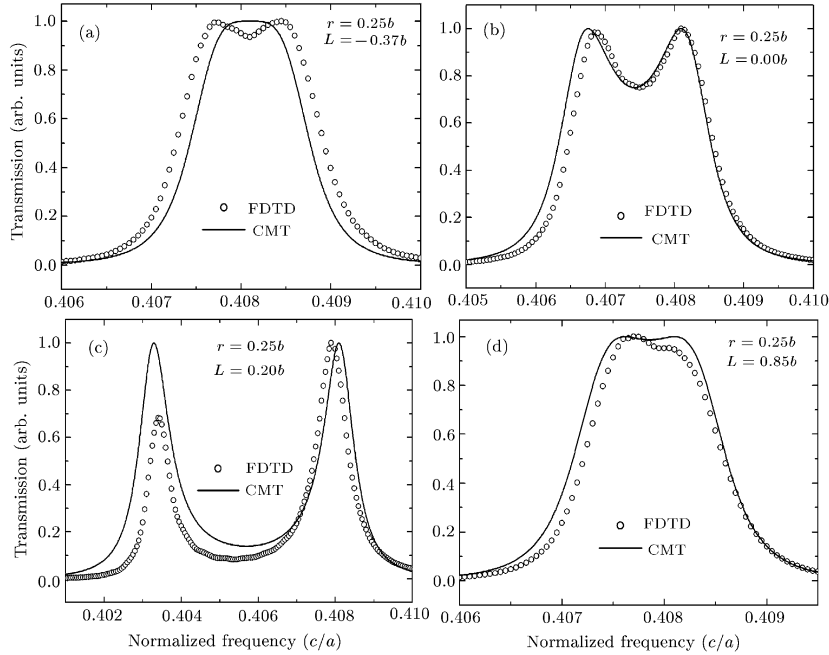
**Fig. 4.** (a) Relationship between the transmission at the valley of the spectra ( $T_0$ ) and the phase shift ( $\varphi$ ) for the three one-dimensional PC molecules studied. (b) Schematic of the two-dimensional PC molecules studied. The two PC atoms forming the PC molecule are indicated by dashed boxes and they are separated by a distance of  $L$ .

shown in Fig. 5 by solid lines. In all the cases, it is found that the results calculated by the CMT are in good agreement with those obtained by the FDTD. This further confirms the validity of our physical model for the coupling of PC atoms.

Now let us focus on the evolution of the transmission spectrum upon the increase in the displacement. In Fig. 5(a), a flat transmission spectrum is observed for  $L = -0.37b$ . The phase shift is estimated to be  $\varphi = 0.50\pi$ . This displacement is intentionally designed to achieve the flat transmission spectrum. In the absence of any displacement ( $L = 0.00b$ ), we can clearly resolve two peaks representing the bonding and anti-bonding states, as shown in Fig. 5(b). At this time, the phase shift is estimated to be  $\varphi_0 = 0.80\pi$ .

As we increase  $L$  to  $0.20b$ , the phase shift is increased to  $0.96\pi$ . The corresponding  $T_0$  in this case is rather small, as shown in Fig. 5(c). If we further increase  $L$  to  $0.85b$ , the phase shift is increased to  $1.50\pi$  and the transmission spectrum becomes flat again. Therefore, it is confirmed that the transmission spectra of the PC molecules can be modified by adjusting

different displacements. The results for displacements of  $-0.37b$ ,  $0.00b$ ,  $0.20b$  and  $0.85b$  are presented in Figs. 5(a), 5(b), 5(c) and 5(d) respectively by open circles. The results calculated by the CMT are also



**Fig. 5.** Evolution of the transmission spectrum of the two-dimensional PC molecule upon the increase in the separation between the two constitutional PC atoms: (a)  $L = -0.37b$ ; (b)  $L = 0.00b$ ; (c)  $L = 0.20b$ ; (d)  $L = 0.85b$ .

the phase shift between the two PC atoms. This provides us an effective way to control the coupling of PC atoms.

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