Engineering the mode parity of the ground state in photonic crystal molecules

Niccolò Caselli,[1,*] Francesca Intonti,[1] Francesco Riboli,[1] and Massimo Gurioli[1]

[1]*European Laboratory for Non-linear Spectroscopy, 50019 Sesto Fiorentino (FI), Italy, and Università degli Studi di Firenze, Dipartimento di Fisica e Astronomia, 50019 Sesto Fiorentino (FI), Italy*

[*]*caselli@lens.unifi.it*

Abstract: We propose a way to engineer the design of photonic molecules, realized by coupling two photonic crystal cavities, that allows an accurate control of the parity of their ground states. The spatial distribution of the fundamental mode of photonic molecules can be tuned from a bonding to an antibonding character by a local and continuous modification of the dielectric environment in between the two coupled cavities. In the systems that we investigate the transition could be experimentally accomplished by post-fabrication methods in either a reversible or an irreversible way. We notably find that the mode parity exchange is tightly related to a dramatic variation of the far field emission pattern, leading to the possibility to exploit these systems and techniques for future applications in optoelectronics.

OCIS codes: (140.3945) Microcavities; (230.4555) Coupled resonators; (260.2160) Energy transfer; (230.5298) Photonic crystals.

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1. Introduction

Dielectric point defects in photonic crystals (PCs) generate localized states for light in the photonic band gaps, similarly to the case of electronic states in the band gap of semiconductor materials [1]. These localized light states play a relevant role in the development of light emitters and optical waveguides [2]. The general properties of the photonic modes in dielectric defects in PCs, also known as photonic crystal cavities (PCCs), are very similar to atomic states. Extending the analogy with quantum mechanics, coupled PCCs are also denominated photonic crystal molecules (PCM) [3–7]. In such systems the molecular-like orbital is achieved by an evanescent tunnelling between each single PCC resonant modes, whenever the frequency matching and spatial overlap between them are fulfilled. The value of the photonic coupling (proportional to the tunnelling rate) is directly measured by the molecular mode splitting at the anticrossing point [7, 8].

Quite remarkably, and differently than in real molecules, in PCMs the sign of the interatomic coupling is not uniquely defined [9–11] and so is the parity of the modes. Recently it has been proved by the analysis of the far field emission that it is possible to change the character of a given PCM mode from even to odd, depending on the lattice direction along which the two PCCs are coupled [11]. Following quantum mechanics denominations, the even molecular state is named the bonding (B) state and it corresponds to the ground state in the case of negative coupling, while the odd molecular state is

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denominated the antibonding (A) state and it is associated to the ground state if the coupling is positive.

Here we address the problem of a fine tuning of the photonic coupling around zero, changing from positive to negative values. The aim of the paper is to demonstrate, by accurate numerical calculations, that it is possible to tune the ground state of a given PCM from a bonding to an antibonding character. This overturn is realized by a local modification of the dielectric environment in between the two coupled cavities, leading to a fine control of the photon tunneling. Moreover we predict that, in peculiar systems, the transition can be achieved by post-fabrication methods, either in a static or in a dynamic way.

2. Numerical characterization of photonic crystal molecules

We consider a 320 nm-thick semiconductor membrane with an index of refraction n = 3.484, the same of GaAs material, but we could have chosen Si or Si_3N_4 as well. The photonic structure is a two dimensional triangular lattice of holes (n = 1) with lattice constant of 308 nm, the pores have a diameter of 193.2 nm, leading to a 35% filling fraction. The single cavity, denominated D2, is formed by four missing holes and with the chosen parameters its fundamental mode is at a wavelength around 1.3 μm [12]. The photonic molecule is considered in the so called K-coupling, which is formed by two PCCs aligned along the principal K-axis of the PC (see Fig. 1(b) for a scheme of the system). 3D numerical calculations were performed with finite-difference time domain (FDTD) solver packages (CrystalWave by Photon Design). The simulated spectrum shows a doublet structure with an energy splitting of the order of 1 meV [11]. Both ground state (GS) and of the first excited state (ES) are almost linearly polarized along the x-direction. The K-coupling has been recently demonstrated to support antibonding GS [11], which is in contrast with the intuitive expectation on the basis of the quantum mechanical analogy. An important consequence of the antibonding mode parity is that the far field emission of the GS is exactly zero along k_x = 0 and in particular at normal direction [11], as a consequence of destructive interference between the two out of phase PCCs [13, 14]. For similar reasons (and in analogy with two slits Young experiment [14]) the even ES has a strong emission along the normal direction, due to the constructive interference of the two in phase PCCs along k_x = 0. Therefore a change in the mode parity and symmetry can determine a large variation in the angular distribution of the out of plane losses for the PCM modes. All these predictions are in good agreement with the experimental data [11].

3. Parity exchange

The character (B or A) of the GS depends on the overlap integral between the two atomic modes weighed over the dielectric function of the photonic system [15]. Recently it has been shown than the fine tuning of the dielectric environment in between the two PCCs allowed to control the photonic coupling [8]. An open question is whether it would be possible to control not only the value but also the sign of the photonic coupling by small modifications in the PCM design in the region of strong overlap of the single PCM modes. As a good approximation, the electric field of B and A molecular modes are given by $\vec{E}_B(\vec{r}) = \vec{E}_0(\vec{r}+\vec{\delta}) + \vec{E}_0(\vec{r}-\vec{\delta})$ and $\vec{E}_A(\vec{r}) = \vec{E}_0(\vec{r}+\vec{\delta}) - \vec{E}_0(\vec{r}-\vec{\delta})$, where $\vec{E}_0(\vec{r})$ is the electric field of the single PCM and $2\vec{\delta}$ is the spatial distance between the two coupled PCMs. Then the spatial distribution of the overlap between $\vec{E}_0(\vec{r}+\vec{\delta})$ and $\vec{E}_0(\vec{r}-\vec{\delta})$ can be obtained by mapping $\left(\left|\vec{E}_B(\vec{r})\right|^2 - \left|\vec{E}_A(\vec{r})\right|^2\right)$, which for K-coupled, D2 based, PCM is given in Fig. 1(a), where the color scale indicates positive (red) and negative (blue) values.

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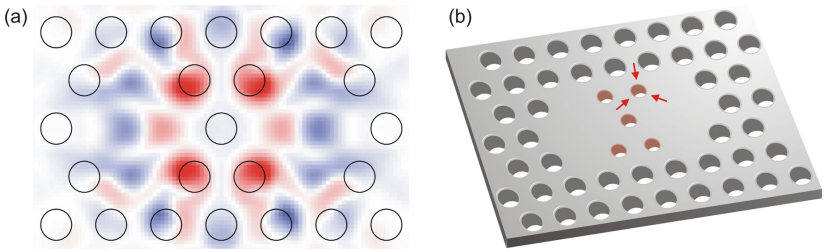

Fig. 1. (a) Map of the quantity $\left(\left|\vec{E}_B(\vec{r})\right|^2-\left|\vec{E}_A(\vec{r})\right|^2\right)$ which gives the mode overlap spatial distribution of the two single PCCs, $\left(\vec{E}_0(\vec{r}+\vec{\delta})\cdot\vec{E}_0^*(\vec{r}-\vec{\delta})+\vec{E}_0^*(\vec{r}+\vec{\delta})\cdot\vec{E}_0(\vec{r}-\vec{\delta})\right)$. Superimposed on the map are reported in black the photonic pores. (b) Scheme of the modified PCM (with the five reduced central pores in red colour) for efficient tuning of the coupling strength between the two PCCs.

The overlap is distributed on the whole system, but it shows the maximum value close to the four pores around the central pore between the two cavities. Then we choose to consider a slight reduction of the diameter of the central holes of the PCM [in particular the five central holes highlighted in Fig. 1(b)], imposing a symmetric perturbation (in order to maintain the zero detuning condition) that can be also experimentally achieved by well developed post-fabrication processes, as the micro-infiltration technique [16].

The photon energy values of the B and A modes of the modified PCM are reported in Fig. 2(a) as a function of the diameter of the five modified holes. Starting from the nominal hole diameter of 193.2 nm, corresponding to an antibonding GS with a 1.0 meV splitting, we see that the diameter reduction produces a continuous decreasing of the photonic coupling. For a modified hole diameter of 183.2 nm we find a single resonant mode, meaning that the photonic coupling is decreased down to a value much below the mode broadening. This leads to an accidental degeneracy of the two modes since the C_{2v} symmetry of the K-coupled D2 photonic cavities, cannot support degenerate modes, accordingly to the group theory [17]. With a further reduction the GS is changed into a bonding character, as a consequence of the change of the photonic coupling sign. For hole diameter of 173.2 nm the splitting between the GS and the ES is of the order of 1 meV, as for the nominal PCM, but their parity is reversed. Therefore a smooth transition from bonding to antibonding GS can be achieved. A more intuitive picture of the physics underlying the data reported in Fig. 2(a) can be obtained by considering the dielectric perturbation induced tuning. Decreasing the hole diameter means adding dielectric material, accordingly with the observed red shift of both modes. In addition, the perturbation being very local, the mode shift is larger the higher is the mode electric field intensity at the dielectric modification. In fact, the quantity $\left(\left|\vec{E}_B(\vec{r})\right|^2-\left|\vec{E}_A(\vec{r})\right|^2\right)$, reported in Fig. 2(a), gives the difference in the electric field intensity between the B and A modes. Therefore increasing the refractive index in the red regions through the local and symmetric perturbation, results in a more pronounced red shift of the B mode with respect to the A mode red shift. In summary, the different red shift of the B and A molecular-like modes gives the transition described in Fig. 2(a).

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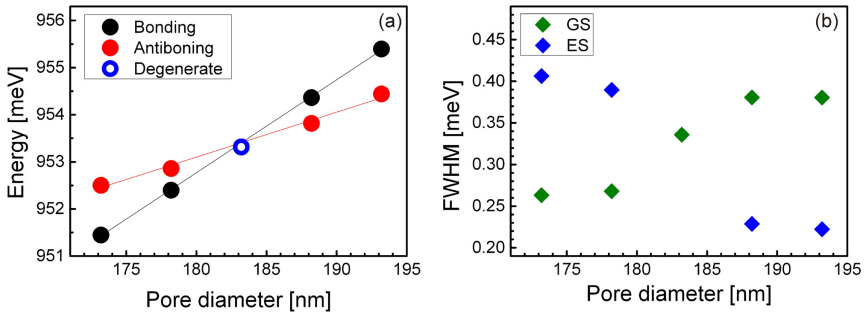

Fig. 2. (a) Peak position of the bonding (B) and antibonding (A) modes as a function of the diameter of the five central pores, calculated with FDTD simulations. (b) Spectral broadening of the GS and ES modes as a function of the diameter of the five central pores, calculated with FDTD simulations.

Further information about the photonic molecular modes parity transition is obtained by analysing the mode Q factors as a function of the hole diameter [Fig. 2(b)]. It is well known that the formation of the molecular modes with opposite parity tailors the diffraction losses [4]. Figure 2(b) reports the mode broadenings of both the GS (green diamonds) and the ES (blue diamonds), as a function of the diameter of the five central pores of the PCM. For the nominal PCM the GS broadening is of the order of 0.38 meV, while a smaller broadening of 0.22 meV is found for the ES, in agreement with the far field patterns [11] that show that the GS has larger diffractive losses than the ES. These values are almost constant when reducing the hole diameter away from the parity inversion, then they reach an intermediate value when the coupling vanishes and finally they are exchanged after the transition. In other words, we found that the Q factors of the A and B modes respectively change very little, and this is not surprisingly since the emissions in the far field [11] are strongly determined by the Young-like interference associated with the mode parities. We also found that the A mode is always broader than the B one, in contrast to the intuitive findings of Ref [4]. for coupled L3 PCCs, associated to the strong (weak) emission of the B (A) mode in the vertical direction. However the discrepancy is only apparent, since both in Ref [4]. and here the broader mode has larger diffractive losses in the light cone. The different behaviour is simply due to the differences in the angular patterns of the single PCC modes, as L3 cavity is compared to the D2 cavity. Therefore the broadening exchange of the GS and ES modes reported in Fig. 2(b) is a consequence of the parity transition achieved with the manipulation of five central pore diameters.

4. Post-fabrication control of parity exchange

It could be questioned whether unavoidable dielectric disorder, associated to the fabrication tolerance, would allow or not to reach the parity tuning up to the targeted control. This should not be a problem, since it is well known that several post-fabrication methods have been developed for compensating fabrication induced dielectric disorder, such as tip [12], carrier injection [18] and thermal tuning [19], wet chemical digital etching [20], atomic layer deposition [21, 22], anodic and laser nano-oxidation [23–25], liquid micro-infiltration [16, 26, 27], and, as a matter of fact, disorder compensated homoatomic and heteroatomic photonic molecules have been realized [7]. At the same time, it could be interesting to explore whether the described methods can be exploited to produce a post-fabrication control of the mode parity in PCMs, which due to the peculiar far field pattern of the A and B mode could be used to realize optical switches.

In order to propose experimental methods to achieve a post-fabrication coupling control of the PCM, we consider a gentle modification of the refractive index within a circular central region of the PCM with a diameter of the order of 0.8 μm. To fix the problem, a controlled reduction of the effective refractive index could be experimentally obtained either by a local

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CW-laser oxidation of the semiconductor slab [24, 25], or dynamically by injecting free carriers in the slab with a fs pulsed laser [18]. In this theoretical analysis we propose to implement such techniques in the case of the modified PCM with the five central hole diameters reduced at 173.2 nm, because starting from such a peculiar geometry we can describe the bonding to antibonding ground state transition, opposite to that due to the PCM design modification, reported in Fig. 2(a). The results are reported in Fig. 3, where the schemes of the modified PCMs (that include the design of the disks of reduced refractive index) are drawn as left panels and the corresponding calculated spectra, with the label indicating the mode parity, are reported in the right panels. Starting from the nominal refractive index equal to 3.484, in which condition the GS is bonding and the splitting between GS and ES is 1.1 meV, we reduce the refractive index of the circular central part of the underlying slab at 3.416. The corresponding calculated spectrum shows a single peak only, denoting a very small (if any) photonic coupling. Eventually for a refractive index of 3.348, we find that the GS character is changed into the antibonding one and that it is energy-split from the B-ES back to 1.2 meV.

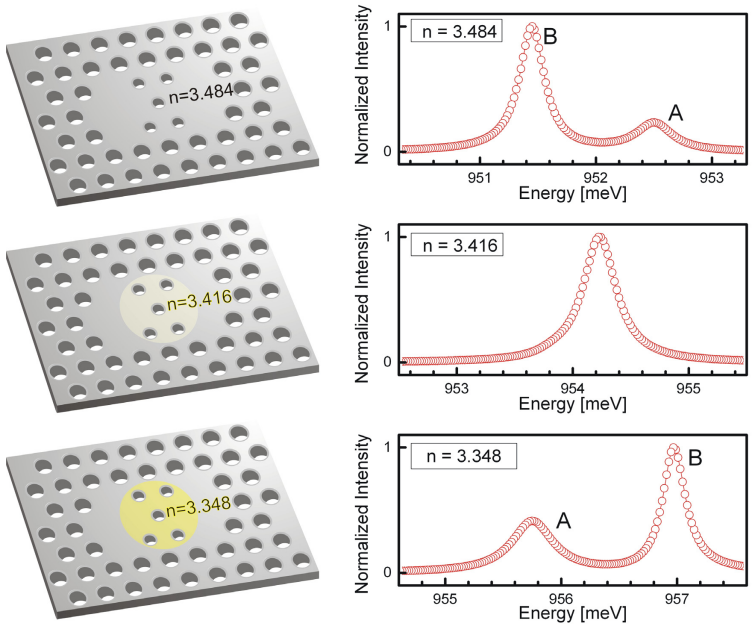

Fig. 3. Left panel: schemes of the modified PCM with the five central pores of the PCM reduced at 173.2 nm. First row, nominal sample with n = 3.484 in the entire slab; second row, reduction to n = 3.416 in the central circular region (pale yellow circle); third row, reduction to n = 3.348 in the central circular region (yellow circle). Right panel: FDTD spectra of the two fundamental modes corresponding to the schemes in the left panel.

5. Summary

In summary, we have theoretically demonstrated that it is possible to tune a photonic molecule mode from the bonding to the antibonding character and vice versa. Following our results, it could be possible to tailor the mode parity, thus controlling the photon evanescent wave of the single PCC mode that constitutes a given PCM. The control can be experimentally achieved by peculiar designing the central region between the two PCCs by irreversible post-fabrication oxidation or even by a dynamic and reversible way by exploiting fs pulsed laser, for instance. We believe that these peculiar properties would open the road to possible applications in quantum optical information processing, including the optical switch of the far field pattern of quantum emitters. In addition, our results can be directly linked to

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the growing interest in quantum simulators based on arrays of PCCs [28, 29]. In the framework of a tight-binding formulation, with an effective intercavity coupling parameter J, the theoretical models so far assumed J to be positive. With our results, we have not only shown that J can be negative but also that it can be continuously tuned around the zero, possibly leading to the development of novel quantum correlation effects.

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