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Manipulation of electronic states and photonic states in nanosilicon

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ABSTRACT

On different size hierarchy, period symmetry provides energy band structure, and symmetry breaking produces localized states in gap, for example nanostructures open electronic band gap by confining electrons, but defects in symmetry system produce localized electronic states in gap. The experimental results demonstrate that controlling localized states in gap by changing passivation environment can manipulate emission wavelength, such as stimulated emission at 700 nm due to oxygen passivation and enhanced electroluminescence near 1600 nm due to ytterbium passivation on nanosilicon. In same way, modulating filling fraction and period parameters in photonic crystal enlarges width of photonic band gap (PBG) by confining photons. Symmetry breaking due to defects is effective in manipulating photonic states. New applications for selecting modes in nanolaser and for building single photon source in quantum information are explored by manipulating and coupling between electronic states and photonic states.

It is interesting in natural sciences that many analogous structures and properties occur on different size hierarchy, for example in nanoscale space related to the de Broglie wavelength of electron and in sub-micrometer scale related to the de Broglie wavelength of photon. Low-dimensional nanostructures for confining electron open band gap and breaking symmetry due to their defect produces localized electronic states in band gap. In same way, modulating filling fraction and period parameters in photonic crystal for confining photon can enlarge width of photonic band gap (PBG). Symmetry breaking due to defects in the lattice is effective in manipulating photonic states. These researches could find some important applications such as a selecting modes device in nanolaser or a single photon source for quantum information [1–8].

For exploring new application of these effects in nanolaser, at first the stimulated emission is obtained on silicon quantum dots (Si QDs) embedded in oxide or nitride, whose wavelength could be manipulated into the window of optical communication by depositing Yb on Si QDs, in which the quantum confinement (QC) effect and the curved surface (CS) effect play main roles [6]. And then a suitably tailored dielectric environment around Si QDs is required for manipulating photonic states [9,10]. Photonic crystals provide resonant cavities for selecting modes of nanolaser, in which it is essential to design crystal structures with PBG as large as possible and to make defect states localize in PBG for coupling the emission [11,12]. In this interesting way, new application in obtaining single photon source is explored, in which single QD for coherent emission is selected by marking on Si QD with characteristic localized states rather than by limiting space for selecting QD. It is fine and novel that defect states localized in PBG is manipulated to couple single QD. In previous work, the CS effect is often submerged in the size effect, which makes some confusion when the QC effect fails for smaller QDs. In manipulating width of PBG, the arising question is for the photon confinement effect and the lattices symmetry breaking effect how to affect photonic states, respectively. In the article, it is a goal to establish the origin and exact mechanism for manipulating electronic states and photonic states on Si QDs and in Si photonic crystals.

Si QDs, embedded in oxide or nitride, are prepared by pulse laser etching (PLE) and pulse laser deposit (PLD) on silicon in various conditions [8]. The laser for PLE is focused on a wafer of P-type silicon placed in nitrogen or oxygen atmospheres. The intensity of the laser pulse is about 5×10^{8} W cm^{-2} on silicon, which is sufficient to produce the plasma vibrating on silicon. Nanostructures are prepared by plasma vibrating to distribute on the wall of the Purcell cavity. Then PLD process builds nitride or oxide layer on the nanosilicon. After rapidly annealing and quenching, the structures with Si QDs embedded in nitride or oxide layer are formed by aggregating of rich silicon.

Photoluminescence (PL) spectra of the samples can be measured under the 514 nm excitation at room-temperature by using RENISHAW Micro-Raman Systems. The sharp PL peaks are observed on samples prepared in nitrogen or oxygen atmospheres, which are kept at some wavelength which is independent on sizes of QDs. It is exciting that they have the threshold behavior and the optical gain on samples [13]. Fig. 1 shows the emission coming from localized states in band gap, in which the stimulated emission center at 693 nm (Fig. 1(a)) may be due to Si$=$O bond and at 604 nm (Fig. 1(b)) is possible coming from

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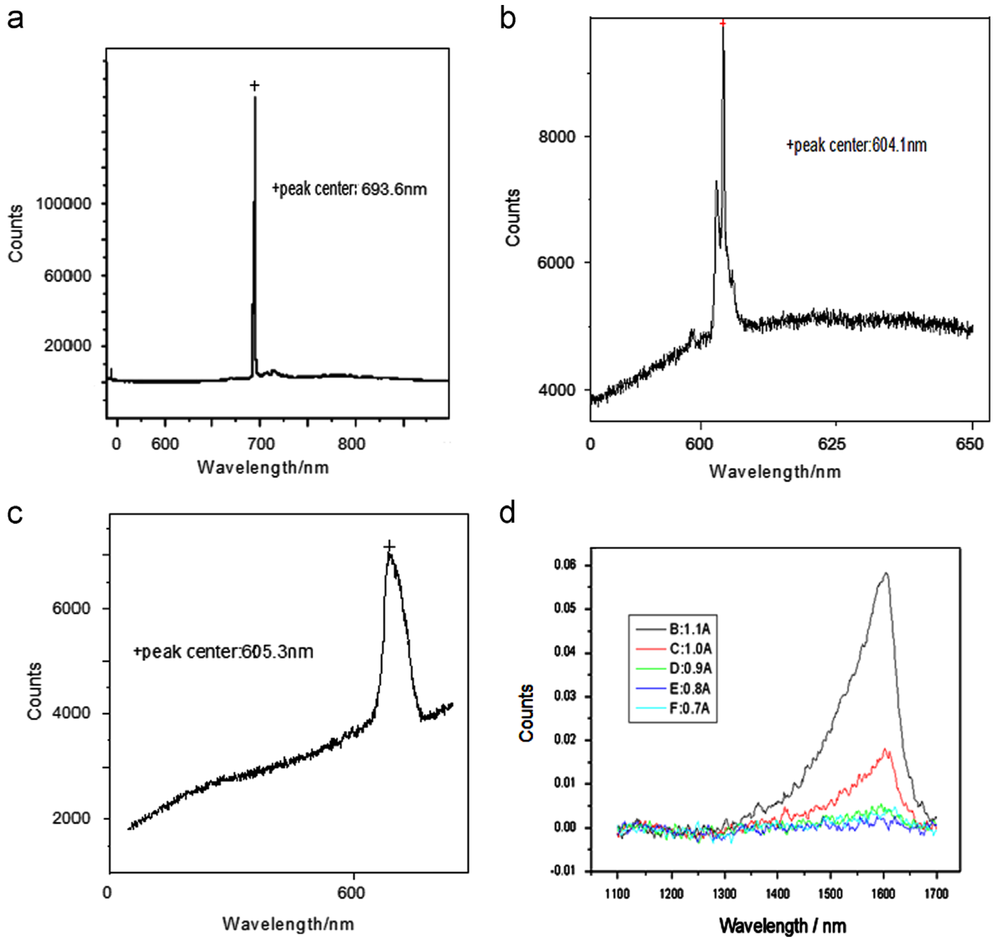

Fig. 1. Manipulation for emission wavelength in PL and EL spectra due to localized states. Stimulated emission at (a) 693 nm and (b) 604 nm for Si QDs prepared in oxygen atmosphere; (c) 605 nm for Si QDs prepared in nitrogen atmosphere; and (d) 1600 nm for Yb deposited on Si QDs prepared by PLD.

Si–O–Si bond on surface of Si QDs. Fig. 1(c) shows a stimulated peak at 605 nm produced from the emission center in nitride layer on Si QDs. The electroluminescence (EL) peaks in optical communication window are observed on the samples in which the Yb ions beam is deposited on Si QDs by PLD, as shown in Fig. 1(d) whose inset indicates that the emission intensity increases with elevation of the pumping current, in which the threshold is about 0.9 A on the sample.

For explaining the emission from localized states, some special surface structures including a facet and a curved surface are built on a Si QDs to compare their density of states. An opened bandgap and a quasi-direct gap structure are obtained for a good passivation of Si–H bonds. Fig. 2(a) shows a Si–Yb bond on the surface with larger curvature, which can provide the localized levels in band gap. But a Si–Yb bond on the facet of Si QDs cannot provide any localized level in gap, as shown in Fig. 2(b). This comparison shows the CS effect on Si QDs. It is clear that larger bond angle on surface of nanostructures related to larger curvature is important to form and manipulate localized states.

In Si QDs system, the level of the electronic states localized in band gap is stated by followed form [6]:

$$E_L = C/r^m - \beta A \tag{1}$$

where β is the bond coefficient, r is the radius of QD and C is the coefficient of QC effect, in which the index m is about 1.7 for Si QDs embedded in oxide. The factor A coming from the simulation calculation involves the surface curvature and the surface systematization as followed: $A = B^{1/(1+d)}/R$, which affects the energy level localizing in gap, where R is the curvature radius of surface, B is the bonding cover factor on surface and index d is cover dimension, such as $d = 0$ for S═O bond, $d = 1$ for Si-O-Si bridge bond and $d = 2$ for Si–N bond or Si–Yb bond. They relate to point, line and film forms of bonding cover on surface, which determine the level position of the localized states in gap. In the formula (1), the first term relates to the QC effect for confining electrons, and the second term presents the CS effect for breaking symmetry from abrupt larger curvature on bonding place of Si QD, which provides the localized levels in band gap. Here, the CS effect obviously brings symmetry breaking in the QD system.

The calculation in the CS effect model for breaking symmetry of Si QD demonstrates an interesting relationship between the energy levels localized in band gap and the bonding angles on surface with different curvatures, for example some Si–O–Si bond with different bonding angle on curved surface produces localized state with different level in band gap. As shown in Fig. 3, it is clear that the smaller bonding angle related to larger surface curvature makes the shifting of localized states to deeper position in band gap on Si QD. It is useful in this way for the states gap ΔE to be manipulated into the window of optical communication by the CS effect.

The CS effect is often submerged in the size effect when the diameter of QDs is smaller than 3 nm [14]. In physical conception the QC effect depends on sizes of Si QDs because of confining electron to increase energy which is described by the first term in the formula (1), but the levels of the localized states slowly arise along with the second term in the formula (1) on smaller Si QDs with sphere shape. As shown in Fig. 4, the QC effect and the CS effect for Si–O–Si bridge bond on spherical QDs are compared, in which the different trends in evolution occur. The elevating of the

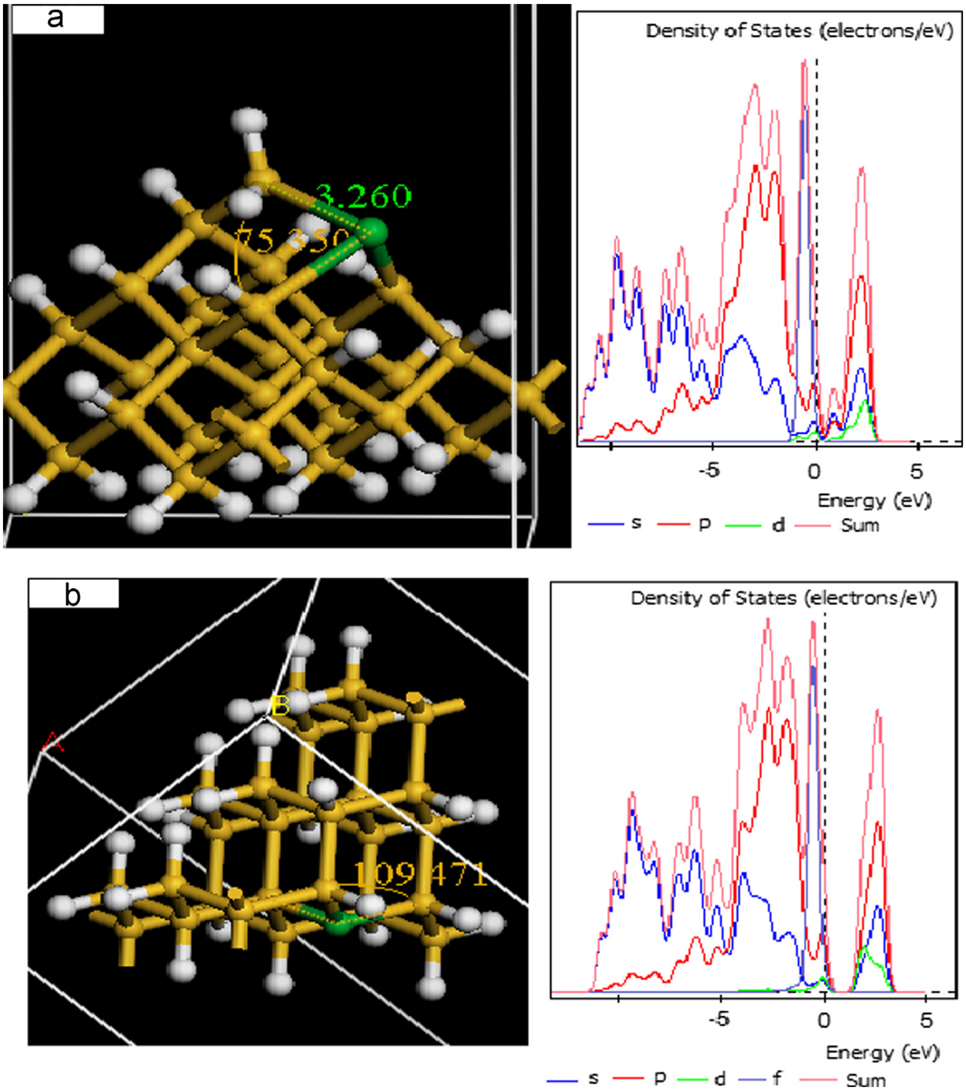

Fig. 2. Si–Yb bond (green color) structures (a) on curved surface and (b) on facet of Si QDs, and their density of states. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

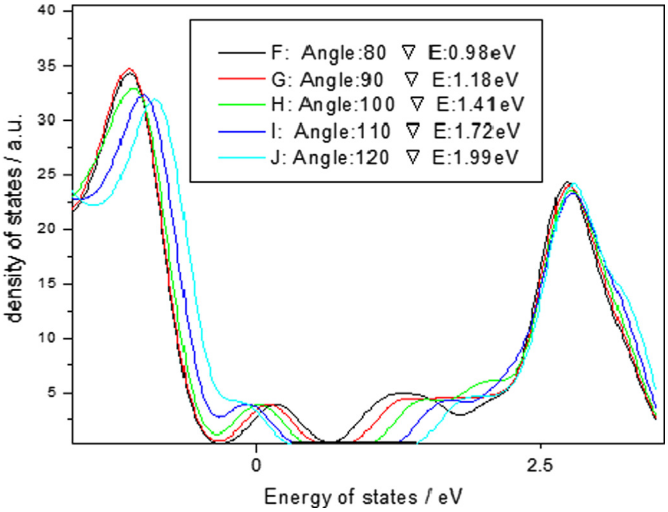

Fig. 3. Relationship between the states localized in band gap and the bonding angles of Si–O–Si bond on different surface of Si QD.

energy levels with decrease of sizes of QDs gets along with the curve B in Fig. 4 due to the QC effect related to the first term in formula (1), and the localized states decline with increase of surface curvature of spherical QDs whose diameters decrease, in which the red dots C in Fig. 4 describe the change of energy levels with various surface curvature in CS effect related to the second term in formula (1). It is noted that the level of the states in CS effect is affected by their bonding curvature on surface rather than their sizes. Finally, the curve D in Fig. 4 provides the realized levels of the localized states involving the QC effect and the CS effect.

In nanolaser, a four energy levels system is built, in which the pumping level sits on conduction band opened by the QC effect, and the population inversion occurs between two groups of localized states produced by CS effect in gap near conduction band and near valence band respectively, for example Si QD passivated by oxygen or nitrogen builds the four energy levels construction. The localized states in gap are manipulated in emission wavelength by CS effect.

Then photonic crystals with cavities or rods lattices are used to select laser modes. It is essential to design lattices structure with a band gap as large as possible and to make defect states localize in photon band gap (PBG) for emission. It is easier to fabricate two-dimensional (2D) PBG structures in this regime. They may bring about some peculiar physical phenomena, as well as wide applications in scientific and technical areas. Here many interesting questions are proposed in the exploring, such as how to enlarge the width of PBG, for changing crystal symmetry or confining

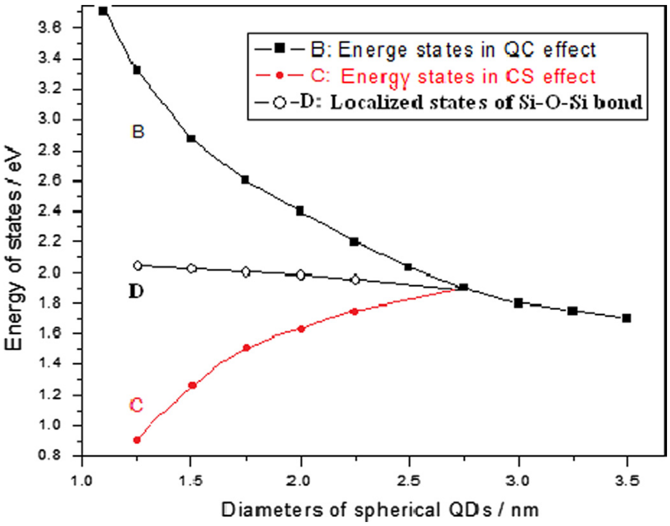

Fig. 4. Comparison between QC effect along with curve B and CS effect along with curve C on Si QDs, in which the final localized states evolve along with curve D. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article).

photons how to affect PBG, and how to manipulate localized states in PBG by changing shape and size of defect in photonic crystals. We try to resolve these problems and study emission on silicon quantum dots embedded in defect of photonic crystals.

The calculation indicates that both increasing symmetry and confining photons in photonic crystals can enlarge width of PBG. In order to change symmetry, we fix period parameter $X=0.4\ \mu m$ and change period parameter Z in $X\times Z$ rectangle array of cavities, in which optimum symmetry occurs at the point with period parameters $X=Z=0.4\ \mu m$ to form square array. On the other hand, confining photons is enhanced with decreasing parameter Z in rectangle array of cavities as well as QC effect. As shown in Fig. 5, the two kinds of different trends build a peak near period parameter $Z=0.4\ \mu m$ along with the PBG width evolution curve. Through simulation calculation, the energy width of PBG is obtained, which is described by followed form:

$$\Delta E=-M(Z-0.4)^2+N/(Z-0.17)+C \tag{2}$$

where simulation parameter M should be larger in the first term of the formula related to the photonic crystal symmetry effect which plays a main role near $Z=0.4\ \mu m$. But M becomes less with far away from point $Z=0.4\ \mu m$, in which the second term plays a main role related to the photon confinement effect instead of the symmetry effect. The simulating calculation indicates that the parabola is good for describing the symmetry effect in photonic crystal, and the inverse proportion curve is suitable for describing the photon confinement effect. It is clear that the two trends are same as $Z>0.4\ \mu m$, but they are inverse as $Z<0.4\ \mu m$.

Fig. 6(a) shows the confining photons structures in cavities array on silicon, in which the space decreases for confining photons and becomes to dots shape from line shape with increasing filling fraction r/a, where a is period parameter and r is radius of cavity. As shown in Fig. 6(b), it is noted that photons field is confined into points shape as filling fraction r/a increases to 0.5. Here, there may be new effect that makes PBG width decline obviously in TM modes because confining space is about 100 nm less than the de Broglie wavelength of photon as filling fraction d/a ($d=2r$) is larger than 0.9. It is interesting that cavities array transfers to rods array structures with increasing filling fraction to some value.

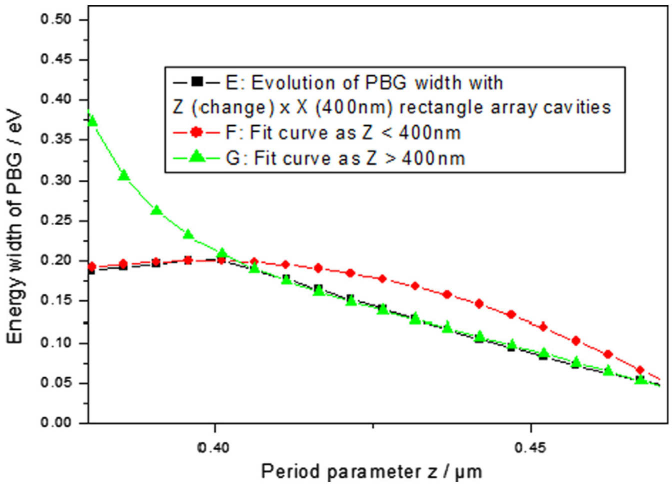

Fig. 5. Evolution of PBG width with changing period z, in which the parabola fit describes the symmetry breaking effect, and the inverse proportion curve is suitable for describing the photon confinement effect.

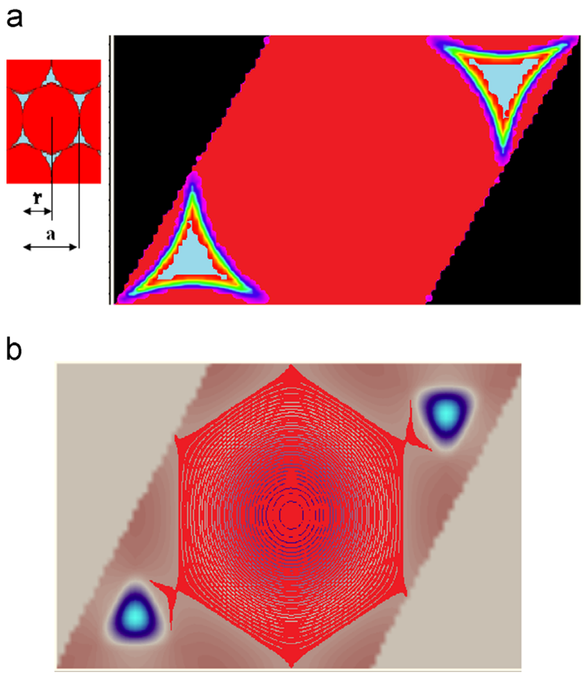

Fig. 6. (a) Confining photons structures in hexagonal cavities array on silicon, in which space of confining photons decreases and becomes to dots shape from lines shape with increasing the filling fraction r/a. (b) Photons field distribution in hexagonal cavities array in simulation calculation, in which blue color region relates to enhanced density of photons. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

Changing filling fraction can manipulate PBG so effective in square and hexagonal lattices of cavities, in which it is clear that enhancing confinement for photons enlarges width of PBG with increasing filling fraction. The photon confinement effect is observed obviously along with evolution curves of PBG center versus filling fraction, as well as the QC effect for electron.

Usually they have different trends, such as reducing crystal symmetry by adding cavities pattern could enhance confinement for photons to open PBG, so the wider PBG originates in the photon confinement effect rather than symmetry reduction in previous work [11].

Defect in photonic crystals breaks symmetry to form localized states in PBG, for example shape and size of H1 defect are modified on 2D hexagonal lattices of cavities to manipulate localized states in PBG, in which the Si QDs plug in the defect cavity. The evolution

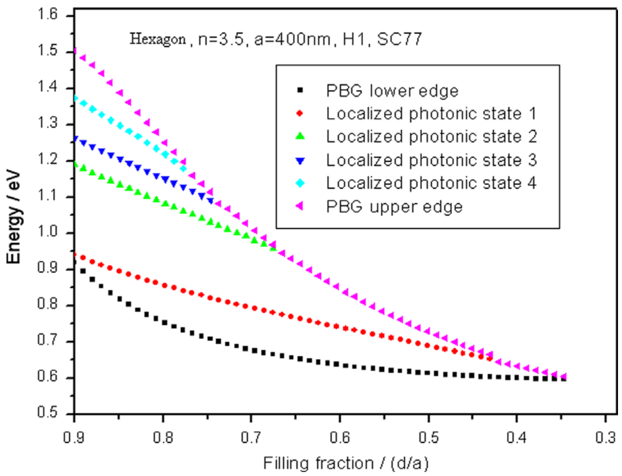

Fig. 7. Evolution of PBG width and localized photonic states in band gap versus filling fraction, in which PBG opens with the photon confinement effect resulting from increase of filling fraction and the localized states slowly elevate in PBG due to defect.

of localized states in PBG with increasing radius of H1 defect cavity is used to manipulate photonic states for coupling to output light in nanolaser. The localized photonic state in PBG and the width of PBG can also be manipulated by changing period parameter a, in which the photon confinement effect plays a main role. In this way, we could select photonic states with some characteristic modes for coupling to output light into the window of optical communication.

What a similar diagram Fig. 7 is, as compared with Fig. 4. Here, as well as QC effect, the photon confinement effect is obviously observed, in which PBG opens with confining photons resulting from increase of filling fraction, and the localized states slowly elevate in PBG due to defect. The characteristic properties of photonic states in photon layer are very like to the electronic properties in nanoscale. It is realized that coupling between electronic states and photonic states is used to select modes and make resonance in nanolaser.

In the way, the single photon source can be obtained, in which single QD marked with the characteristic localized states produced from surface defect on QD can be selected by coupling the localized photonic states in PBG rather than by limiting space of single QD. The coupling can transfer traversing photons into vertical photons from amplifying spontaneous emission to improve single photon emitting.

In conclusion, we can prepare Si QDs by PLE and PLD and manipulate emission wavelength in various passivation environment by the QC effect and the CS effect. On smaller Si QDs, nanostructures can be activated in oxygen or nitrogen for emission, and the emission wavelength is manipulated into the window of optical communication by Si–Yb bonds. As well as in nanoscale, in sub-microscale the photon can be manipulated by confining photon and changing symmetry in photonic crystals, in which many new phenomena are discovered, such as modifying symmetry parameters and making defects affect the photonic manipulation. Here, both the quantum confinement effect in nanoscale for electron or in sub-microscale for photon and the breaking symmetry effect play main roles in manipulating emission on silicon nanostructures embedded in photonic crystals, which have new applications in nanolaser for integrating on silicon chip and single photon source for quantum information.

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