

# Strain Profile and Size Dependent Electronic Bandstructure of Type-I CdS/CdSe Quantum Ring

Sumanta Bose\*, W. J. Fan† and D. H. Zhang‡

*School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore*

*OPTIMUS, Centre for OptoElectronics and Biophotonics, Nanyang Technological University, Singapore*

*LUMINOUS! Centre of Excellence for Semiconductor Lighting & Displays, Nanyang Technological University, Singapore*

\*sumanta001@e.ntu.edu.sg, †ewjfan@ntu.edu.sg, ‡edhzhang@ntu.edu.sg

**Abstract**—We study the strain profiles of Type-I CdS/CdSe quantum ring (QR) using the Valence force field method with Keating potential. The strain affects its electronic bandstructure which is calculated for varying QR widths using an effective mass envelope function theory based 8-band  $k\cdot p$  model. This is followed by an electron-hole charge distribution study of the QR.

**Index Terms**—Quantum Ring, Strain Profile, Valence Force Field, Electronic bandstructure,  $k\cdot p$  method, Charge density

## I. INTRODUCTION

Quantum rings (QRs) are a very recently developed class of nanoparticle in which a traditionally used active material with lower bandgap (e.g. CdSe) forms a ring around a traditionally used barrier material with higher bandgap (e.g. CdS). The ring may be rectangular [1] or toroid-like [2], depending on the synthesis techniques. Recently, Fedin *et al.* have demonstrated the colloidal synthesis of luminescent CdSe QRs via controlled etching of nanoplatelets (NPLs) [2]. Fig. 1 shows a schematic of a typical rectangular Type-I core/crown CdS/CdSe QR. Owing to the non-trivial topology of semiconductor QRs, they exhibit interesting optoelectronic properties. They have high optical tunability and their emission characteristics can be spectrally tuned by varying the extent of lateral confinement. Delikanli *et al.* have shown that the Type-I core/crown CdS/CdSe QRs of a particular thickness is capable of exhibiting a range of peak emission wavelengths – from that of core only CdS NPLs to that of core only CdSe NPLs having the same thickness [1]. These CdS/CdSe QRs have already found application as phosphor for color conversion in white light LEDs [1]. They are also potential candidates for magneto-optical device applications (using Aharonov-Bohm effect) [2]. To understand the physics of the QRs for such applications, it is important to study how-and-why its electronic structure can be tailored by varying their lateral confinement. In this work, we will study the electronic structure along with strain profile and charge density for QRs of varying ring widths.

## II. THEORETICAL MODEL

We have studied CdS/CdSe QRs in the zincblende phase. For each QR, we use an effective mass envelope function theory approach based on the 8-band  $k\cdot p$  model to obtain its electronic structure in the vicinity of the  $\Gamma$ -point. The 8-band Hamiltonian for the strained QR can be simply written

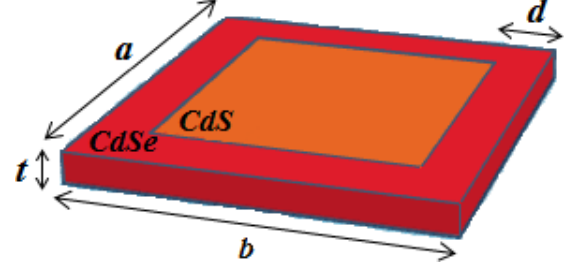


Figure 1. Schematic of a typical Type-I core/crown CdS/CdSe quantum ring of dimensions  $a \times b \times t$  and crown width  $d$ .

as  $H = H_k + H_{so} + \Phi_{QR}$ , where  $H_k$  is the kinetic effective-mass component for the interaction between the conduction bands (CB), valence bands (VB) and the spin-orbit coupling, and  $H_{so}$  is the valence band spin-orbit coupling Hamiltonian [3].  $\Phi_{QR}$  is the confining potential of the QR. The electronic structure is affected by the strain induced in the QR system due to hydrostatic and sheer influences. To calculate the strain, we model the interatomic interactions using the Valence force field (VFF) method with Keating potential. The strain is a resultant of the system's strain-energy-minimized final state. The expressions for the Hamiltonian terms, strain energy and other material parameters can be referred to in our previous works [3], [4].

## III. RESULTS AND DISCUSSION

In this work, we have studied Type-I square CdS/CdSe QRs with  $a = b = 12$  nm,  $t = 4$  monolayers (ML) = 1.2 nm with varying  $d = 2.4, 1.8$  and 1.2 nm. Fig. 2 shows the strain profile distributions for  $\epsilon_{xx}$ ,  $\epsilon_{yy}$  and  $\epsilon_{zz}$  in the (001) plane for QR with  $d = 2.4$  nm. For a strained layer, the CB edge is shifted by  $\delta E_c = a_c(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$ , while the VB heavy-hole ( $hh$ ) and light-hole ( $lh$ ) edge are shifted by  $\delta E_{hh} = (a_v + 0.5b)(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) - 1.5b\epsilon_{zz}$  and  $\delta E_{lh} = (a_v - 0.5b)(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + 1.5b\epsilon_{zz}$ , where  $a_c$ ,  $a_v$  and  $b$  are the hydrostatic deformation potential for CB and VB, and sheer deformation potential respectively [5]. In Fig. 2, the warmer colors (reddish) represent tensile strain ( $\epsilon_{\parallel} > 0$ ), while cooler colors (bluish) represent compressive strain ( $\epsilon_{\parallel} < 0$ ). Tensile strain causes the CB and VB band-edges to come closer ( $\delta E_c < 0$  and  $\delta E_{hh}, \delta E_{lh} > 0$ ), while compressive strain has the inverse effect.

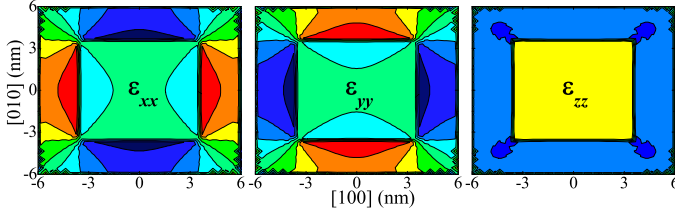


Figure 2. Strain profile distribution ( $\epsilon_{xx}$ ,  $\epsilon_{yy}$  and  $\epsilon_{zz}$ ) in the (001) plane of the 12 nm–4 ML CdS/CdSe QRs with  $d = 2.4$  nm cut horizontally along the center. Warmer colors (reddish) represent tensile strain, while cooler colors (bluish) represent compressive strain. QR width and core dimensions are mentioned.

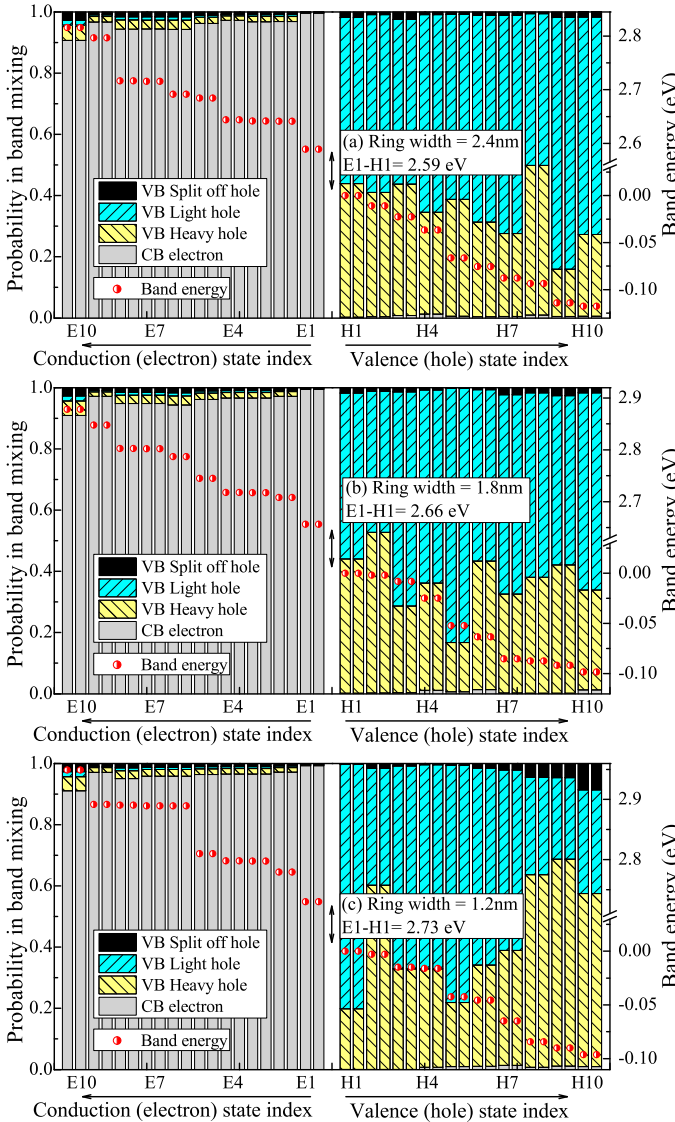


Figure 3. Electronic bandstructure and the probability in band mixing between conduction electrons and valence heavy-, light- and split off holes for 12 nm–4 ML CdS/CdSe QRs with  $d =$  (a) 2.4 nm, (b) 1.8 nm, and (c) 1.2 nm. E1–H1 transition energies are indicated. Legends show the band mixing probabilities.

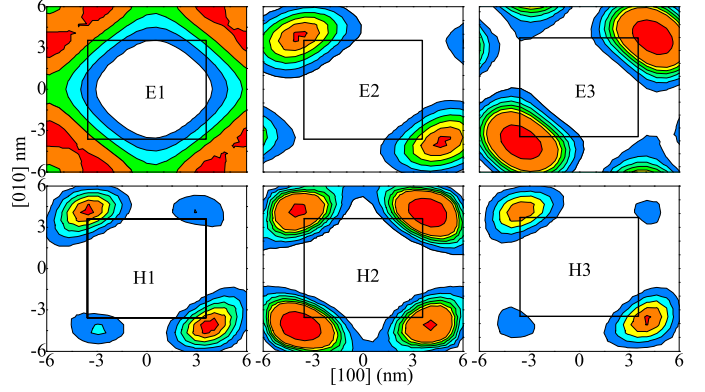


Figure 4. Spatial charge density of the first three electron (E) and hole (H) states of the 12 nm–4 ML CdS/CdSe QRs with  $d = 2.4$  nm in the (001) plane cut horizontally along the center of the QR. Warmer (reddish) colors depict higher occupation probability over cooler ones (bluish). QR dimensions are mentioned. The inner box depicts the CdS core which is  $7.2 \text{ nm} \times 7.2 \text{ nm}$ .

We note that, for  $\epsilon_{xx}$  there is tensile strain along the [100] direction, and compressive strain along the [010] direction. With the same analogy, for  $\epsilon_{yy}$  there is tensile strain along the [010] direction, and compressive strain along [100] direction. However, for  $\epsilon_{zz}$  there is purely compressive strain in the QR. All components of the strain tensor ( $\epsilon_{ij}$ ) affect the electronic bandstructure and other optoelectronic properties as they are included in the Hamiltonian elements [4].

Now, with the strain effects consideration along with the interactions of CB with VB [ $hh$ ,  $lh$ , and split-off ( $so$ ) holes], we have calculated the electronic bandstructure of the Type-I core/crown 12 nm–4 ML CdS/CdSe QRs, with  $d = 2.4, 1.8$  and  $1.2$  nm. This is shown in Fig. 3, along with the band mixing probabilities of CB electrons with VB  $hh$ ,  $lh$  and  $so$  holes. Here, we show the first ten conduction (E) and valence (H) states. The E1–H1 is the CB to VB band-edge gap, i.e. the exciton transition energy. With decreasing ring width (frames a to c in Fig. 3), they experience greater quantum confinement, so the E1–H1 transition energy rises. However, the intraband state gaps decrease. As the ring width decreases from 2.4 nm to 1.2 nm, we notice that  $\Delta(E1-E10)$  decreases from 227 meV to 219 meV, and so does  $\Delta(H1-H10)$  from 117 meV to 96 meV.

Moreover, the contribution of  $lh$  in H1 and  $hh$  in H2 increases as the ring becomes thinner. But, at large the contributions of  $lh$  are much more when compared to conventional NPLs [4].

Fig. 4 shows the spatial charge densities of the first three electron and hole states (square of the wavefunction  $|\Psi|^2$  i.e. probability of finding them), of the 12 nm–4 ML CdS/CdSe QRs with  $d = 2.4$  nm in the (001) plane. The charge density of electrons is primarily concentrated in the active CdSe QR region of lower bandgap, while the probability of finding electron in the high bandgap CdS core is negligible. Similarly for holes, they are also pocketed largely in the QR corners. This facilitates effective electron-hole wavefunction overlap and efficient excitonic recombination for photon emission.

#### IV. SUMMARY AND CONCLUSION

We have calculated and shown the strain components,  $\epsilon_{xx}$ ,  $\epsilon_{yy}$  and  $\epsilon_{zz}$  in Type-I CdS/CdSe QRs and considered its effect on the electronic structure. Using the 8-band  $k \cdot p$  method and considering electron and  $hh$ ,  $lh$  and  $so$  hole interaction, we have calculated the electronic bandstructure. With decreasing ring width the quantum confinement increases and the effective E1–H1 gap increases, while the intraband state gaps decrease. The electron and hole spatial charge densities are primarily concentrated in the low bandgap active CdSe ring, enabling effective overlap and excitonic recombination.

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