Type-II Quantum Dot Nanowire Structures with Large Oscillator Strengths for Optical Quantum Gating Applications

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***Abstract*—The exciton oscillator strength (OS) in type-II quantum dot (QD) nanowires is calculated by using a fast and efficient method. We propose a new structure in Double-Well QD (DWQD) nanowire that considerably increases OS of type-II QDs which is a key parameter in optical quantum gating in the stimulated Raman adiabatic passage (STIRAP) process [1] for implementing quantum gates.**

I. Introduction

In nanowires, crystal phase QDs can be synthesized by modifying the crystallographic structure. This structuring can be made with atomic monolayer precision that allows precise control of QDs in nanowires thus forming attractive systems for engineering QD-based functionalities such as quantum gates. The crystallographic interfaces usually feature type II-band alignment where electrons and holes are spatially separated in the different polytypes which is a key asset in implementing quantum gates. However, it also leads to very small OS in these structures compared to type-I QDs.
In this work, we calculate exciton OS of QD nanowire structure shown in Fig(1a) using a full configuration interaction (CI) description of the few particle electron-hole system. Whereas widely used methods such as ab initio or tight binding are numerically demanding, the CI method is more efficient and thus suitable for engineering and design of quantum devices. We show that engineering a nanowire in the DWQD configuration, the OS is increased up to 10 times compared to single-well QDs (SWQD).

II. Modeling Coulomb Interaction By CI Method

The exciton Hamiltonian can be expressed as:

$$\hat{H} = \hat{H}_h + \hat{H}_e + \hat{H}_c, \tag{1}$$

where $\hat{H}_{(e/h)}$ is the single-particle Hamiltonian for the electron/hole written as:

$$\hat{H}_k = -\frac{\hbar^2}{2m_k}\nabla^2 + V_T^k(R,\theta) + V_{QW}^k(z), \tag{2}$$

in the effective mass approximation in cylindrical coordinates. Here $k \in e,h$ is a subscript denoting the electron or hole respectively, m_k is the effective mass that we assume to be constant in the whole system; ∇ is the 3D laplacian; the first term in (2) is the kinetic energy of the electron (hole); $V_{QW}^k(z)$ is the confinement potential for the electron (hole) along the growth direction for the single-well band structure shown in Fig(1b), and $V_T^k(R,\theta)$ is the in-plane confinement potential which we approximate by a hard-wall potential.
$\hat{H}_c$ in (1) is the Coulomb interaction between electron and hole. The representation of this operator in terms of creation and annihilation operators is:

$$\hat{H}_c = \frac{1}{2}\sum_{nm}\int\int \frac{q^2}{4\pi\epsilon}\frac{\hat{\psi}_m^\dagger(r)\hat{\psi}_n^\dagger(r')\hat{\psi}_n(r')\hat{\psi}_m(r)}{|r-r'|}drdr'. \tag{3}$$

Here, q is the unit electronic charge; ε is the permittivity of material; $\hat{\psi}_{(m/n)}(r)$ is the electron/hole field operator, respectively, at position $r:(R,\theta,z)$. This few-particle Hamiltonian containing the electron-hole interaction is expanded within the basis of the energetically lowest electron and hole single-particle states in the conduction and valence bands. Then, the exciton state is obtained by direct diagonalization of the full Hamiltonian.
We calculate the OS of the exciton in the ground state which is a central parameter in the study of optical transitions [2] and in realizing qubit operations [1] given by:

$$OS = \frac{2|p_{cv}|^2}{m_0\hbar\omega_0}|\int \Psi_{exc}(r,r)dr|^2, \tag{4}$$

where m_0 is free electron mass and p_{cv} is the interband momentum matrix element. Fig(2) shows the dependence of the calculated normalized OS on NW length. The OS gets fixed at around 100nm length of NW and doesn't change much in NWs longer than 100nm. Also we see that the normalized OS is quite small (4%) in these structures compared to a typical type-I QD which could approach 100%.

III. Improving OS by engineering DWQD structure

For improving OS in type-II structures we propose the DWQD structure shown in Fig (3a). In this structure we find electron states to be localized in QDs. Most hole states are localized in the outer surrounding material of the QDs in the NW, but there are a few hole states mainly localized in the

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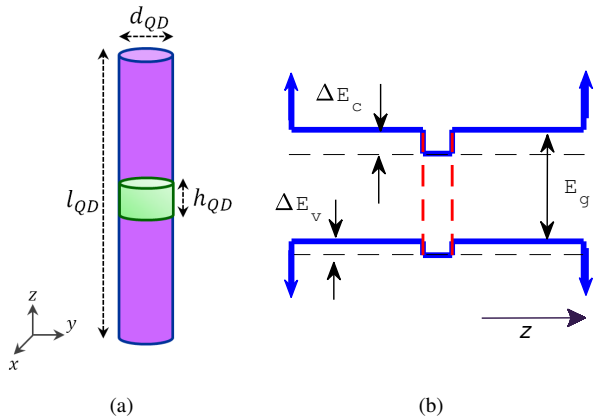

Fig. 1: a) Type-II single-well QD nanowire b) its band-edge energy along the z direction. Band structure parameters used in our calculation are: $\Delta E_c = 0.129eV, \Delta E_v = 0.0646eV, E_g = 1.474eV, m_e = 0.068m_0, m_h = 0.64m_0$.

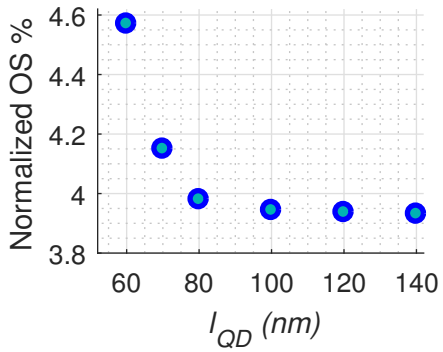

Fig. 2: Ground state exciton normalized OS ($OS/OS_0 \times 100, OS_0 = \frac{2|p_{cv}|^2}{m_0\hbar\omega_0}$)in SWQD structure as a function of l_{QD}. In this calculation: $d_{QD} = 20\ nm, h_{QD} = 4\ nm$.

inner surrounding material. Fig (3c) displays single-particle ground state electron and lowest energy confined hole state in the conduction and valance band, respectively.

Fig (4) shows how the normalized OS of the lowest-energy state bound exciton state changes as a function of the distance between the two QDs in the nanowire. We see at some I values an OS in the DWQD which is 10 times larger than the OS in the SWQD shown in Fig (2) .

ACKNOWLEDGMENT

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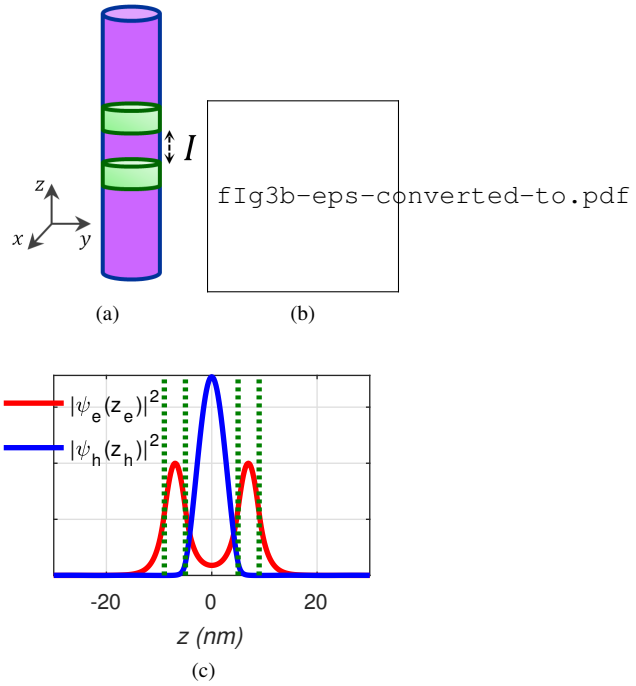

Fig. 3: a) Type-II DWQD nanowire b) the band-edge energy along the z direction c) ground state probability density along the growth direction for electron in the conduction band and for the lowest-energy confined hole state in the valence band. $l_{QD} = 60\ nm, h_{QD} = 4\ nm, d_{QD} = 20\ nm$.

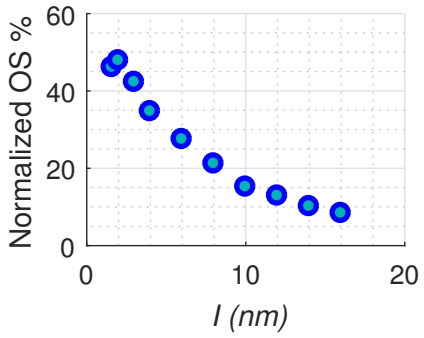

Fig. 4: Ground state exciton normalized OS ($OS/OS_0 \times 100, OS_0 = \frac{2|p_{cv}|^2}{m_0\hbar\omega_0}$) in DWQD structure as a function of I. In this calculation: $d_{QD} = 20\ nm, h_{QD} = 4\ nm$.