

5.1 INTRODUCTION

Semiconductor Quantum Dots (QDs) have gained increasing attention of scientists and engineers of various disciplines due to their flexible tunability and unique properties [107]. For a number of optoelectronic applications, e.g., light emitting diodes (LEDs), photovoltaic cells, semiconductor nanocrystals, and quantum dots (QDs) have large surface-to-volume ratio, which is beneficial for photoluminescence efficiency. The confinement of light-generated charge carriers at surface states of QDs can be used to supplement QDs in solar cells for obtaining high efficiency. The band gaps, optical transitions, and chemical properties, etc., of QDs are tunable using the pseudopotential approach.

CHAPTER 5

Investigated Optical Studies of Si Quantum Dot

Different quantum dot solar concentrators are discussed in the literature [111]. Kennedy *et al.* [112] have devoted the low optical efficiencies for single-plate Quantum Dot Solar Concentrators (QDSCs) are due to low photoluminescent quantum yields and large overlap between Quantum Dot (QD) emission and absorption spectra of present commercially available visible emitting QDs. Also, they showed that using Near Infra-Red (NIR) emitting QDs, re-absorption of QD emitted photons can be reduced greatly, thereby diminishing escape cone losses thus improving optical efficiencies and concentration ratios. It is shown that, escape cone losses using Monte-Carlo ray trace modelling account for ~5% of incident photons absorbed in QDSCs containing commercially available visible emitting QDs. Gallagher *et al.* [113] have described a novel non-tracking concentrator, which uses nano-scale quantum dot technology to render the concept of a Fluorescent Dye Solar Concentrator (FSC) a practical proposition.

They mentioned that the Quantum Dot Solar Concentrator (QDSC) comprises Quantum Dots (QDs) seeded in materials are suitable for incorporation into building facades, and have found that Photo-voltaic (PV) cells attached to the edges convert direct and diffuse solar energy collected into electricity. Meanwhile, they have fabricated small scale LED devices. Also, Gallagher *et al.* [114] have been undertaken spectroscopic measurements for a range of different Quantum Dot (QD) types and transparent host materials, and proved that high transparency in the matrix material and QDs with high quantum efficiency is essential for an efficient QDSC. They determined an

5.1 INTRODUCTION

Semiconductor Quantum Dots (QD's) have gained increasing attention of scientists and engineers of various disciplines due to their flexible processibility and unique properties [107]. For a number of optoelectronic applications, e.g., Light Emitting Diodes (LED) [108], strongly luminescent semiconductor nanocrystals are highly desirable. However, due to the large surface-to-volume ratio of nanoparticles, the most common reason for poor luminescence efficiency is nonradioactive recombination of light-generated charge carriers at surface-traps [109]. It is fantastic to implement QD's in solar cells for obtaining high efficiency and green energy applications. So, band gaps, optical constants, photoemission spectra, dielectric functions depending on frequency and wave vector, alloy properties, bonding and chemical properties, etc. have been evaluated for many materials using the pseudopotential approach [110].

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optimum matrix material for a QDSC based on absorption characteristics and an optimum commercially available QD type has been chosen using steady-state absorption, photoluminescence and photoluminescence excitation spectroscopy of QDs in solution and solid matrices.

Udipi *et al.* [115] presented semi classical simulation results for the potential energy profile and electron density distribution in 200 nm silicon quantum dot. For the solution of the continuity equation, the efficient difference approximations, proposed by Scharfetter and Gummel [116] extended to three dimensions. In essence, they followed the two-dimensional approach due to Selberherr *et al.* [117] extend two to three dimensions. Zhong and Liu [118] have presented theoretical calculations of the scattering intensity for the Electron Raman Scattering (ERS) process associated with the bulk like Longitudinal Optical (LO) and Interface Optical (IO) phonon modes in GaAs/Ga_{1-x}Al_xAs Quantum Dots (QDs), additionally to their study the selection rules for these processes and the singularities in the Raman spectra for various concentrations (x). Hasaneen *et al.* [119] had been described a model to simulate the electrical characteristics of non-volatile floating gate quantum dot memory cells. They computed the tunnelling rate of electrons using the transition Hamiltonian of Bardeen and calculated the wave functions and potential energies of the quantum well channel and quantum dot gate using a self-consistent numerical solution of Schrödinger and Poisson equations.

They showed that by changing the quantum dot charge, the resistor values can be changed by 40%. Experimentally, Schmidt *et al.* [120] produced effectively buried quantum well dots on the basis of InGaAs/GaAs single quantum wells using high resolution electron beam lithography and selective wet etching of the top barrier. They generated Dot structures with diameters down to 20 nm and maintained high luminescence efficiencies down to the smallest sizes. Also, they observed a blue shift of up to 9 meV for 23 nm quantum dots. The investigation of new materials research is interesting when one tries to gain some information about the diameter dependence of the compounds. It seems more fundamental to relate the diameter dependence behaviour to the bonds between nearest atoms. By controlling the evolution with diameter dependence of the compound, it could attempt to link the effect of dot diameter to the quantum dot potential. In this context, we have used this procedure for testing the validity of our model [121] of QD's potential. The aim of this paper is to extend this method for calculating the diameter dependence on QD's potential for dot diameters down to 52 nm using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) and to investigate the optical properties of Si.