CHAPTER 8

First-Principles Calculations for Optical Investigations of PbX (X=S, Te) Compounds under Quantum Dots Diameter Effect

8.1 INTRODUCTION

The IV–VI semiconductors in semiconductor periodic table are among the most interesting materials in solid state physics. The most widely studied compounds in this group are PbS and PbTe. These materials have narrow band gap, which is usually less than 0.5 eV, which has positive temperature coefficient dEg = dT, and high electron mobility [167]. These lead salts has interesting optoelectronic applications [168]. It is advantageous in using the computational method based on total energy calculations to study the phase transition from the coordinated number Nc = 4 to 6 fold [158]. Third generation approaches to photovoltaics (PVs) aim to decrease costs and significantly increase efficiencies while maintaining the economic and environmental cost advantage of thin film deposition techniques [159]. There are several approaches to achieve such multiple energy threshold devices [160]; tandem or multicolor cells, concentrator systems, intermediate level cells, multiple carrier excitations, up/down conversion and hot carrier cells [169].

Billaud and Truong [170] have computed the ground state Lamb shift of a semiconductor spherical quantum dot in the effective mass approximation. It appears to be significant enough to be detectable for a wide range of small quantum dots synthesized in semiconductors. They have suggested the Casimir effect to observe it. While, Thu and Voskoboynikov [171] have calculated the lowest energy states of electrons confined in an asymmetrical InAs/GaAs double lens-shaped quantum dot molecule in external magnetic field. Based on the effective three-dimensional one electronic band Hamiltonian approximation, the electronic energy states of the system were computed by non-linear iterative method using Comsol MultiPhysics package. This description allows them to simulate the semiconductor quantum dot molecule in arbitrary directed magnetic field. Simulation results clearly have shown that, the diamagnetic shifts of the electronic energy levels are anisotropic and non-uniform.

Therefore, they have demonstrated an opportunity to dynamically manipulate electronic states not only by varying the magnitude but also changing the direction of the magnetic field. Moreover, Lam and Ng [172] have applied this as bio tags to emit different color light with different dot sizes, and quantum dots are currently extensively studied for application as quantum devices taking advantage of the artificial atom properties such as their discrete energies, electron spins and quantum transport energies. The self-assembled semiconductor quantum dots are grown on the wetting

layer of a few monolayer thicknesses and subsequently capped with a strain-reduction layer covering the dots to stabilize them. They have studied the indium arsenide/gallium arsenide self-assembled quantum dots modeled with a wetting layer between the quantum dot and substrate, and the strain-reducing capping layer above the quantum dot.

They have introduced a new model with an interfacial layer between the quantum dot and the capping layer and investigate the effective mechanical and electronic properties using the finite element method and deformation potential theory. However, Udipi et al. [115] have 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] have extended to three dimensions. In essence, they have followed the two dimensional approach in accordance to Selberherr et al. [117] which extend two to three dimensions.

Further research on material becomes more interesting ones observe the diameter dependence of the compounds; especially when it is proved with some of other materials [173]. It seems more fundamental to relate the diameter dependence behavior to the bonds between nearest atoms. By controlling the evolution with diameter dependence of the compound, it could attempt to link the effect of quantum dot diameter to the quantum dot potential. In this context, we have used this procedure for testing the validity of our model [121] of QDs potential. The acquired energy band gaps are used to calculate the quantum dot potential and to predict materials for QDs.

The aim of this work is to verify our model [121] for calculating the diameter dependence on QDs potential for dot diameters down to 60 nm and 65 nm for PbS and PbTe compounds respectively using the Full Potential Linearized Augmented Plane Wave (FP-LAPW), in addition to investigating the optical properties of refractive index and optical dielectric constant using specific models for the mentioned alloys.

8.2 CALCULATIONS

The calculations were carried out using full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K code [125]. The exchange correlation potential was treated using the Generalized Gradient