CHAPTER 7

ab initio Method of Optical Investigations of $\text{Cds}_{1-x}\text{te}_{x}$ Alloys under Quantum Dots Diameter Effect

7.1 INTRODUCTION

The main feature of each solar cell is its capability to absorb effectively wide spectrum of photons contained in solar radiation, reaching its active surface. This feature depends on intrinsic optical and electronic properties of semiconductor material, and the critical parameter related to semiconductor is energy band gap and energy band structure. Among available thin-film solar cell (α-Si, $CuInGaSe_2$ and CdTe) materials, cadmium telluride (CdTe) may be the strongest candidate for high throughput, large-scale manufacturing [156] of polycrystalline thin-film solar cells. Because of its high absorption coefficient (> 1 × 104 cm-1) and direct band-gap (1.5 eV), about 1 μm thick CdTe film is enough for absorption of ~90% of photons with energy higher than its band gap. However, the availability of elemental Te may be a concern if production levels increase above 20 GW per year [157]. It is advantageous to use 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 but maintaining the economic and environmental cost advantages 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.

Yum *et al.* [161] have demonstrated PbS:Hg Quantum Dots Sensitized Solar Cell (QDSC) combined with a Dye Sensitized Solar Cell (DSC) to harvest panchromatic solar spectrum from the visible light to the near IR. They have used the filter to split the solar energy and access the total conversion efficiency. The DSC performing 12.4% under AM1.5G sunlight was able to generate 9.1% with a short-wave pass filter cutting off photons of wavelength longer than 650 nm. On the other hand, QDSC performing 5.58% generated 3.42% with the use of a long wave pass filter transmitting beyond 630 nm. Calculated based on transmitted light, DSC and QDSC performed 24.0% and 5.90%, leading to almost 13.1% of estimated total power conversion efficiency by harvesting the solar energy from visible light to the NIR. While, Badawi *et al.* [162] have studied the photovoltaic performance of CdTe Quantum Dots (QDs) Sensitized Solar Cells (QDSSCs) as a function of tuning the band gap of CdTe QDs size. Presynthesized CdTe QDs of radii from 2.1 nm to 2.5 nm were deposited by direct adsorption (DA) technique onto a layer of TiO_2 nanoparticles (NPs) to serve as sensitizers for the solar cells. The characteristic parameters of the assembled QDSSCs were measured under

AM 1.5 sun illuminations. The values of current density (J_{sc}) and overall efficiency (η), increase along with decreasing CdTe QDs size since the Lowest Unoccupied Molecular Orbital (LUMO) levels shifts closer to vacuum level, which causes an increase in the driving force. Furthermore, the photocurrent response of the assembled cells to ONOFF cycles of the illumination indicates the prompt generation of anodic current. Moreover, Emin et al. [163] have reviewed the recent progresses in various quantum dot solar cells that are prepared from colloidal quantum dots. They have discussed the preparation methods, working concepts, advantages and disadvantages of different device architectures. Major topics include integration of colloidal quantum dots in: Schottky solar cells, depleted heterojunction solar cells, extremely thin absorber solar cells, hybrid organic inorganic solar cells, bulk heterojunction solar cells and quantum dot sensitized solar cells. 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] extended to three dimensions. In essence, they have followed the two-dimensional approach due to Selberherr *et al.* [117] extend two to three dimensions.

The investigation of further materials research is interesting on the mark that one tries to gain some information about the diameter dependence of the compounds; especially it is proved with some of the materials [164]. 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 obtained energy band gaps are used to calculate the quantum dot potential and to predict materials for QD's. The aim of this paper is to verify our model [121] for calculating the diameter dependence on QDs potential for dot diameters down to 57 nm, 58 nm and 60 nm for $CdS_{0.75}Te_{0.25}$, $CdS_{0.5}Te_{0.5}$ and $CdS_{0.25}Te_{0.75}$ alloys, respectively using the Full Potential Linearized Augmented Plane Wave (FP-LAPW), in addition to investigate the optical properties of refractive index and optical dielectric constant using specific models for the mentioned alloys.