CHAPTER 6
Further Optical Properties of Cdx (X=S,Te) Compounds under Quantum Dot Diameter Effect: *Ab initio* Method

6.1 INTRODUCTION

Since II-VI semiconductor compounds from the semiconductor periodic table have large optical gap, the feasibility of green blue optoelectronic devices and solar cells has been demonstrated [142]. A wide range of electronic properties of binary compounds has been predicted using theoretical calculations. Different attempts [143] have been made using different models. An experimental and theoretical results comparison may allow testing different competing theoretical approximations. The transition from the coordinated number Nc = 4 to 6 is well demonstrated by the use of a computational method based on total energy calculations [144].

Miguez *et al.* [145] had calculated the binding energies of shallow donors and acceptors in a spherical GaAs-Ga_1-xAl_x as quantum dot under the combined effect of isotropic hydrostatic pressure and an intense laser. They computed the binding energy as a function of hydrostatic pressure, dot sizes and laser field amplitude. They showed and found that, the impurity binding energy increases with pressure, decreases with the laser field amplitude and the pressure effects are more dramatic for donor than acceptor impurities, especially for quantum dots with small radii, respectively. $In_{0.5}Ga_{0.5}As$ Quantum Dots (QD's) stacked structures were studied using Atomic Force Microscopy (AFM), High-Resolution X-Ray Diffraction (HR-XRD) and Photo Luminescence (PL) characterization by Aryanto *et al.* [146]. They evaluated the dots size and dots density in the stacked structures and found them to be strongly influenced by the dot formation in the under layer and the structure of the spacer layers.

However, the dots formation as they researched is not vertically aligned since HR-XRD measurement gave different satellite peaks on n-stacked QD structures, additionally is also attributed to the size, composition and density of the dots in the stacked structures. While, Panchal *et al.* [147] had reviewed research works on silicon Quantum Dots (Si-QDs) embedded in the silicon nitride (SiNx) dielectric matrix films with different fabrication techniques and different characteristics. They discussed the advantages of SiNx as a dielectric compared to silicon dioxide (SiO_2) for Si-QDs from a device point of view, and summarized the fabrication techniques along with different optimized deposition conditions. 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.

Recently, Liu *et al.* [148] synthesized the center hollow ZnO and TiO_2 nanotubes arrays by chemical etching ZnO nanorods and sol-gel process assisted by ZnO nanorods templates, respectively. Furthermore, as an application of the ZnO and TiO_2 nanotubes, they successfully fabricated and characterized the Dye-Sensitized Solar Cells (DSSC's) and the cell performance, respectively. They got an efficiency of DSSC's based on ZnO (1.2%) and TiO_2 (2.1%) nanotubes. Das and Sokol [149] have successfully synthesized nano size zinc oxide (ZnO) at low temperature solution method. Also, they performed the structural characterization, size and distribution of synthesized ZnO particles using X-Ray Diffraction (XRD) and neutron scattering technique. The hybrid polymer-metal oxide bulk heterojunction solar cell fabricated by blending ZnO and regioregular poly (3-hexylthiophene) (P3HT) through solution process and flow coating on a flexible substrate. They have concluded that the decrease in the Photo Luminescence (PL) emission intensity of more than 79% for ZnO: P3HT composites film indicates high charge generation efficiency. The cell shows a V_{oc} and I_{sc} of 0.33 V and 6.5 mA/cm2, respectively. The performance and stability of the cell were investigated using UV illumination of white light.

Finally, Badescu and Badescu [150] have analyzed a system of improving solar cell efficiencies by up-conversion of sub-band-gap light to increase solar cell efficiency. The system involves adding to the cell a so-called up-converter, which is a device able to convert the low-energy (sub band gap) incident solar photons into photons of higher energy. Their main novelty consists of taking into account appropriately the refractive index of solar cell and converter materials. They concluded as follows: (1) The maximum solar energy conversion efficiency increases in case of the Cell and Rear Converter (C–RC) system as compared to the efficiency of a solar cell operating alone, especially at higher values of the concentration ratio; (2) The solar energy conversion efficiency of the C–RC system increases by increasing both the cell and the up-converter refractive indices; (3) The energy conversion efficiency does not increase by adding a front up-converter to the cell, whatever the value of the concentration ratio is.

The investigation of further materials research is interesting when one tries to gain some information about the diameter dependence of the compounds; especially it is proved with some of the materials [151]. It