Electronic Properties of Electron and Hole in Type-II Semiconductor Nano-Heterostructures

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Abstract. In this project, we record the orbitals of electron and hole in type-II (CdTe/CdSe/CdTe/CdSe) semiconductor nanocrystal using effective mass approximation. In type-II the band edges of both valance and conduction band are higher than that of shell. So the electron and hole get confined in different layers of the hetero-structure. The energy eigen values and eigen functions are calculated by solving Schrodinger equation using finite difference matrix method. Based on this we investigate the effect of shell thickness and well width on energy and probability distribution of ground state (1s) and few excited states (1p,1d,etc). Our results predict that, type-II quantum dots have significant importance in photovoltaic applications.

INTRODUCTION

The recent developments in the manufacturing and growth technology have caused the fabrication of the low dimensional systems, which are called nanostructures. Reducing the size of components to the nanoscale (e.g., in nano-heterostructures) gives rise to new possibilities. Quantum dots (QDs) are nanostructures made of semiconductor materials that are small enough to exhibit quantum mechanical properties. Specifically, its charge carriers are confined in all three spatial dimensions [1]. In quantum dots the band energies are dependent on crystal size due to the quantum size effects. This enables band-offset engineering in nanoscaleheterostructures. The modern advances in semiconductor technology allow the preparation of more complex structures such as multiple quantum rings, complex quantum wires and the quantum dot quantum well (QDQW) structures. Heterostructures make it possible to solve the more general problem of controlling the fundamental parameters of semiconductor devices such as bandgaps, effective masses of the charge carriers and the mobilities, refractive indices, electron energy spectrum, etc. Quantum confinement (QC) leads to formation of an ordered set of orbitals at discrete energy levels on the conduction and valance bands in semiconductor quantum dots (QDs), which enables strongly size-dependent control of optical properties.

Quantum dot-quantum wells (QDQW) containing multiple shells have been investigated to seek superior structural properties allowing for strain reduced band engineering. Thus various material and structure combinations have been studied. Core/shell heterostructures are usually divided into two categories, type-I and type-II, depending on the relative alignment of conduction and valence band edges of the materials that are combined at the heterointerface[2]. Recently, Sahin et al.[3] investigated the shell structure and orbital ordering of CdSe/ZnS/CdSe multi-shell quantum-dot quantum-well hetero-nanocrystals. In this project we investigate the orbitals of electron as well as hole in Type-I and Type-II semiconductor nanocrystals. Here we recording the orbitals of both electron and hole in CdTe/CdSe/CdTe/CdSe core/shell/well/shell quantum dot hetero-structures are studied by varying layer thicknesses.

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