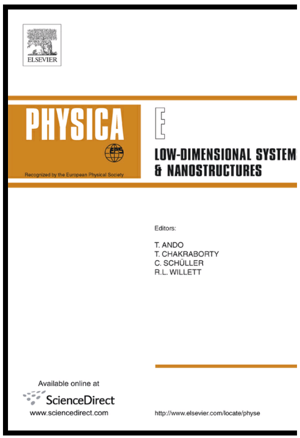
www.elsevier.com/locate/physe

The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X= InN, $In_{0.33}Ga_{0.67}N$) core/shell/shell quantum dot quantum well–A theoretical study

P. Ganesan, L. Senthilkumar

PII: S1386-9477(15)30108-9
DOI: http://dx.doi.org/10.1016/j.physe.2015.07.002
Reference: PHYSE12024

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 10 April 2015
Revised date: 3 July 2015
Accepted date: 6 July 2015

Cite this article as: P. Ganesan and L. Senthilkumar, The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X= InN $In_{0.33}Ga_{0.67}N$) core/shell/shell quantum dot quantum well–A theoretical study *Physica E: Low-dimensional Systems and Nanostructures* http://dx.doi.org/10.1016/j.physe.2015.07.002

The influence of interfaces and intra-band transitions on the band gap of CdS/HgS and GaN/X (X= InN, $In_{0.33}Ga_{0.67}N$) core/shell/shell quantum dot quantum well – A Theoretical study

P. Ganesan and L. Senthilkumar*

Department of Physics, Bharathiar University, Coimbatore, Tamil Nadu, INDIA

Abstract

A theoretical model is presented to calculate the 1s-1s transition energy of an exciton in spherically layered semiconductor Quantum-Dot Quantum-Well (QDQW), based on the LCAO variational method using effective mass approximation. The confinement energies of electron and hole and the Coulombic interaction energy between them are calculated for CdS/HgS/CdS, GaN/X/GaN$\left(X = InN, In_{0.33}Ga_{0.67}N\right)$ (QDQW) with core/shell/shell structures. The results of the proposed model effectively accommodates the polarization effects at the interfaces of different semiconductor materials in a core/shell/shell structure and elucidates the significant influence of interfaces on the band gap with consistency among previous theoretical and experimental results. The wave function of exciton studied shows significant differences with other theory. The change in the band gap of QDQW is attributed to the exciton excitations by thermal occupation of the lowest dark exciton states at different temperatures. In addition, based on Quantum Confined Stark Effect (QCSE) the effect of high electric field on the charge carriers and the corresponding changes in the band gap has been investigated. The applied electric field provides strong overlap between the electron and hole wave functions as well as increases the binding energy of the exciton, which eventually decreases the band gap.

Keywords: excitons, quantum-dot quantum-well, LCAO variational method, Interface roughness, Intersub-band transition, Quantum Confined Stark Effect (QCSE).

[*] **Corresponding Author**

Email: lsenthilkumar@buc.edu.in