Optical Properties of an Indium Doped CdSe Nanocrystal: A Density Functional Approach

Salini K[1)], Thomas Mathew[1, 2)] and Vincent Mathew[1, a]

[1]*Department of Physics, Central University of Kerala, Riverside Transit Campus, Kasaragod, Kerala*
[2]*Department of Physics, St Pius X College Rajapuram, Kasaragod, Kerala*

[a)] Corresponding author: vincent@cukerala.ac.in

Abstract. We have studied the electronic and optical properties of a CdSe nanocrystal doped with n-type impurity atom. First principle calculations of the CdSe nanocrystal based on the density functional theory (DFT), as implemented in the Vienna Ab Initio Simulation Package (VASP) was used in the calculations. We have introduced a single Indium impurity atom into CdSe nanocrystal with 1.3 nm diameter. Nanocrystal surface dangling bonds are passivated with hydrogen atom. The band-structure, density of states and absorption spectra of the doped and undopted nanocrystals were discussed. Inclusion of the n-type impurity atom introduces an additional electron in conduction band, and significantly alters the electronic and optical properties of undoped CdSe nanocrystal. Indium doped CdSe nannocrystal have potential applications in optoelectronic devices.

INTRODUCTION

Semiconductor quantum dots (QDs) acquired much attention over the last two decades due to their size tunable electronic and optical properties. When the size of the QD is smaller than the exciton Bohr radius, the energy levels are discrete due to quantum confinement. There is much effort to create and study the QD due to their potential application in laser [1], light emitting diodes [2], etc. Impurity doping in a bulk semiconductor revolutionized the electronics and semiconductor technology. The properties of a quantum dot can also be tuned by proper impurity doping. Doping with magnetic impurity atom, especially Mn doping in nanocrystal have been studied [3]. By using tightbinding theory and hydrogenic-like impurity model the electronic property of a strongly confined metal-doped nanocrystal were studied [4].

Our earlier calculations were based on the effective mass approximation and considered only the columbic interaction between the charge carriers [5]. DFT is the most successful theory for electronic structure calculations by including proper exchange correlation. In this paper, we conduct a density functional theory (DFT) simulation of a small 1.3 nm CdSe quantum dot doped with single n-type Indium atom. The surface dangling bonds of the nanocrystal are passivated with covalently bonded hydrogen atoms. The simulation provides information on the structural, electronic and optical properties of the QD.

COMPUTATIONAL DETAILS

We have performed the first principle calculations using density functional theory within the VASP package on MedeA platform [6]. The solutions are obtained via projector augmented wave (PAW) method with the plain wave basis set. The structure optimization was carried out by density functional theory including the exchange correlation approximated by generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE). The calculation was carried out with 25 A^0 supercell geometry with the nanocrystal placed at the center of the cell. The plane wave

International Conference on Condensed Matter and Applied Physics (ICC 2015)
AIP Conf. Proc. 1728, 020191-1–020191-4; doi: 10.1063/1.4946242
Published by AIP Publishing. 978-0-7354-1375-7/$30.00