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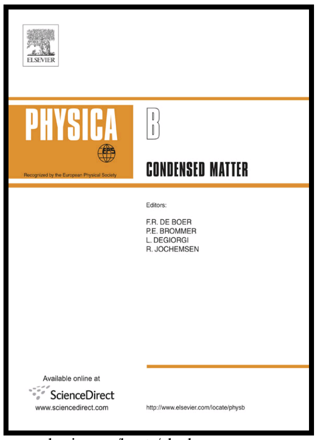

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Stokes shift and fine structure splitting in composition-tunable $Zn_xCd_{1-x}Se$ Nanocrystals: Atomistic tight-binding theory

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Abstract

I report on the atomistic correlation of the structural properties and excitonic splitting of ternary alloy $Zn_xCd_{1-x}Se$ wurtzite nanocrystals using the sp^3s^* empirical tight-binding method with the description of the first nearest neighbouring interaction and bowing effect. Based on a successful model, the computations are presented under various Zn compositions (x) and diameters of alloy $Zn_xCd_{1-x}Se$ nanocrystals with the experimentally synthesized compositions and sizes. With increasing Zn contents (x), the optical band gaps and electron-hole coulomb energies are improved, while ground electron-hole wave function overlaps, electron-hole exchange energies, stokes shift and fine structure splitting are reduced. A composition-tunable emission from blue to yellow wavelength is obviously demonstrated. The optical band gaps, ground electron-hole wave function overlaps, electron-hole interactions, stokes shift and fine structure splitting are progressively decreased with the increasing diameters. Alloy $Zn_xCd_{1-x}Se$ nanocrystal with Zn rich and large diameter is the best candidate to optimistically be used as a source of entangled photon pairs. The agreement with the experimental data is remarkable. Finally, the present systematic study on the structural properties and excitonic splitting predominantly opens a new perspective to understand the size- and composition-dependent properties of $Zn_xCd_{1-x}Se$ nanocrystals with a comprehensive strategy to design the optoelectronic devices.

Keywords: Tight-binding theory, $Zn_xCd_{1-x}Se$, alloy, nanocrystals, stokes shift, fine structure splitting ;

1. Introduction

As an exceptional realization of the semiconductor nanocrystals, semiconductor nanocrystals can act as the alternative candidates in a broad range of applications such as optoelectronic devices [1, 2, 3, 4], solar cells [5, 6, 7, 8], chemical sensors [9] and biological labels [10, 11, 12, 13] owing to their unique structural and optical properties. A general methodology to directly tune the absorption spectrum is accessible through changing the size of the