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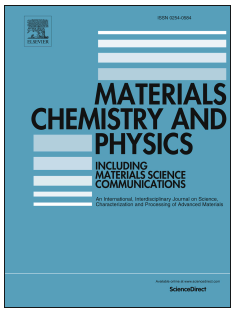

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Theoretical investigation of the structural, optical and magnetic properties of Mn doped and (Mn, Cr) co-doped CdS in its cubic structure

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Abstract

The electronic, magnetic and optical properties of doped CdS:Mn and co-doped CdS:Mn,Cr cubic structures were studied via Density Functional Theory and subsequently compared with the properties of undoped CdS. The doped compound presents semiconducting character similar to the undoped CdS, while the co-doped compound exhibits half metallic properties with a high spin polarization at the Fermi energy. The magnetic moments as well as the trend of magnetic exchange parameters of CdS:Mn and CdS:Mn,Cr, have been analyzed, in addition to the dielectric functions, by starting from calculated density of states for spin polarized configurations. The calculated absorption coefficients lead to direct information on the spectral energy distribution in the range of optoelectronic applications. The optical band gaps of doped and co-doped compounds are higher as compared to the undoped CdS, making the first compounds more interesting for possible technological applications for high density magneto-optical recording.

Keywords: DFT, DMS, transition metal, semiconductor, optoelectronics, half-metallic, CdS

1. Introduction

In the last decade, the II-VI semiconductors become materials of increasing importance for a wide range of applications. With their wide band gap and convenient optical properties, they found applications in spintronics and

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