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Electronic , Optical and Magnetic Properties of low concentration Ni doped CdSe by First Principle Method

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Electronic, Optical and Magnetic Properties of low concentration Ni doped CdSe by First Principle Method M. Yaseen,1, M. Dilawar1, H. Ambreen1, U. Shahid1, Misbah2, M. K. Butt1, A. Ghaffar1, and W. Ren3 1Department of Physics, University of Agriculture, Faisalabad 38040, Pakistan 2Department of Chemistry, University of Agriculture , Faisalabad 38040, Pakistan 3Electronic Material Research Laboratory, Key Laboratory of the Ministry of Education and International Center for Dielectric Research, Xi an Jiaotong University, Xi an 710049, China.Corresponding Author: myaseen_taha@yahoo.com

In this work, electronic, optical and magnetic properties of low concentration Ni doped CdSe was studied systematically by Wien 2K code. Calculations were performed for the band structure in the spin up and down channels, total density of states (TDOS) and partial density of states (PDOS). The Spin-polarized band structure showed that Cd0.9375 Ni0.0625 Se, Cd0.875 Ni0.125 Se and Cd0.75 Ni0.25Se are half metallic ferromagnetic in nature with direct band gap, when the concentration of the transition metal increases the band gap is also increased. In optical properties, we discuss about absorption coefficient, optical conductivity, refractive index, real and imaginary part of dielectric function. Analyzed magnetic properties of Ni doped CdSe compound offers the magnetic moment which indicates the magnetic properties due to d orbital of Ni atoms. Obtained results revealed that Cd1-xNix Se is a suitable and potential candidate for the spintronics and optoelectronics devices.

Key word: Density functional theory; Optical properties, Dilute magnetic semiconductor

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