

Spin-Polarized Investigation of Ferromagnetism on Magnetic Semiconductors $Mn_xCa_{1-x}S$ in the Rock-salt Phase

Authors : B. Ghebouli, M. A. Ghebouli, H. Choutri, M. Fatmi, L. Louail

Abstract : The structural, elastic, electronic and magnetic properties of the diluted magnetic semiconductors $Mn_xCa_{1-x}S$ in the rock-salt phase have been investigated using first-principles calculations. Features such as lattice constant, bulk modulus, elastic constants, spin-polarized band structure, total and local densities of states have been computed. We predict the values of the exchange constants and the band edge spin splitting of the valence and conduction bands. The hybridization between S-3p and Mn-3d produces small local magnetic moment on the nonmagnetic Ca and S sites. The ferromagnetism is induced due to the exchange splitting of S-3p and Mn-3d hybridized bands. The total magnetic moment per Mn of $Mn_xCa_{1-x}S$ is $4.4\mu_B$ and is independent of the Mn concentration. The unfilled Mn -3d levels reduce the local magnetic moment of Mn from its free space charge value of $5\mu_B$ to $4.4\mu_B$ due to 3p-3d hybridization.

Keywords : semiconductors, Ab initio calculations, band-structure, magnetic properties

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