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Study of Structural, Elastic, Electronic and Magnetic Properties of Ga0.875Cr0.125P

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Abstract

We investigate the structural, Elastic, Electronic and Magnetic properties of Ga1-xCrxP diluted Magnetic Semiconductor (x=0.125) in Zinc Blende (B3) phase. The calculations have been performed using Density functional theory as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms code using local density approximation as exchange-correlation (XC) potential. Analysis of electronic structures and magnetic properties show that Ga0.875Cr0.125P diluted magnetic semiconductors has stable half-metallic ferromagnetic nature with 100% spin polarization. The calculated values of s-d exchange constant Nα and p-d exchange constant Nβ shows the magnetic nature of these compounds. These compounds are predicted to good candidate for spintronic applications. Calculated results are in good agreement with previous theoretical and experimental data.