## MS34-P04 | DFT Studies of Structural, Electronic and Magnetic Properties of InP and In0.75X0.25P (where X=Cr, Mn & Fe)

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We investigate the structural, Electronic, Magnetic and Elastic properties of $Ga_{1-x}Cr_xP$, $Ga_{1-x}Mn_xP$ and $Ga_{1-x}Fe_xP$ diluted Magnetic Semiconductor (x=0.25) 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. The study of electronic structures and magnetic properties show that doping of Cr/Mn/Fe transition metal atom in GaP results the induction of ferromagnetism and develops a half metallic (HM) gap at fermi level with 100% spin polarization. The calculated values of s-d exchange constant $N_o\alpha$ and p-d exchange constant $N_o\beta$ indicate 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.