

Investigations of Structural, Electronic, and Half-metallic Ferromagnetic Properties in $(\text{Al, Ga, In})_{1-x}\text{M}(x)\text{N}$ ($\text{M} = \text{Fe, Mn}$) Diluted Magnetic Semiconductors

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Résumé: We investigate the structural, electronic, and magnetic properties of $(\text{M} = \text{Fe, Mn})$ -based zinc blende diluted magnetic semiconductors (DMS) $(\text{Al, Ga, In})_{1-x}\text{M}(x)\text{N}$ for $(x=0.0625, 0.125, 0.25)$, using first-principles calculations with the full-potential linearized augmented plane waves (FP-LAPW) method within the density functional theory and local spin-density approximation. The analysis of electronic structures and magnetic properties show that $(\text{Al, Ga, In})_{1-x}\text{Fe}(x)\text{N}$ at $(x=0.0625, 0.125, 0.25)$ are magnetic insulators, and $\text{In}_{1-x}\text{Mn}(x)\text{N}$ at $(x=0.0625, 0.125)$ are metallic in nature. On the other hand the $(\text{Al, Ga})_{1-x}\text{Mn}(x)\text{N}$ at $(x=0.0625, 0.125, 0.25)$ and $\text{In}_{0.75}\text{Mn}_{0.25}\text{N}$ are half-metallic ferromagnets with magnetic spin polarization of 100 %, where the ferromagnetic ground states result from a double-exchange mechanism, and these compounds are predicted to be good candidates for spintronic applications.