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

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Abstract/Résumé : We investigate the structural, electronic, and magnetic properties of (M = Fe, Mn)-based zinc blende diluted magnetic semiconductors (DMS) (Al, Ga, In)(1-x) M (x) 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 (Al, Ga, In)(1-x) Fe (x) N at (x=0.0625,0.125,0.25) are magnetic insulators, and In1-x Mn (x) N at (x=0.0625,0.125) are metallic in nature. On the other hand the (Al, Ga)(1-x) Mn (x) N at (x=0.0625,0.125,0.25) and In0.75Mn0.25N 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.

Keywords/Mots cléfs :

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