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Half-metallic ferromagnetism in Al1-xCrxP and superlattices (AlP)n/(CrP)m by density functional calculations

Abstract

Using the first-principles full-potential linear muffin-tin orbital (FP-LMTO) method based on density functional theory, we have investigated the electronic structure and magnetism of order dilute ferromagnetic semiconductor $Al_{1-x}Cr_xP$ ($x = 0.125$, 0.25 and 0.50) and the superlattices $(AlP)_1/(CrP)_1$ and $(AlP)_3/(CrP)_1$. For the exchange-correlation functional, the generalized gradient approximation (GGA) has been used. It is shown that these compounds are half-metallic ferromagnets. Calculations of the s-d exchange constant $N_0\alpha$ and p-d exchange constant $N_0\beta$ clearly indicate the magnetic nature of these compounds. We observe that p-d hybridization reduces the local magnetic moment of Cr from its free space charge value and produces small local magnetic moments on the non-magnetic Al and P sites.

Keywords; DMSs, Superlattices, Electronic structure, Magnetic properties