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Résumé :

Electronic and magnetic properties of diluted $B_{1-x}Mn_xN$ alloys are calculated by means of the full potential linearized augmented plane wave (FP-LAPW) method and the generalized gradient approximation (GGA). A half-metallic state is predicted for a composition of 6.25%. The spin majority being metallic and minority being semiconducting. We found a total magnetic moment of 2 μ_B (Bohr-magnetons) per supercell, in agreement with the half-metallic behaviour. The main contribution of the cell magnetic moment is localized at the transition metal site Mn, with a local moment of 1.24 μ_B.