# Magnetic properties of CaN, SrN, and BaN

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Spintronic applications require the use of ferromagnetic materials for spin injection and detection. Several classes of magnetic semiconductors have been considered thus far. Magnetism in these systems stems from the presence of transition metal or rare earth ions with the half-filled spin-polarized *d* or *f* shells. On the other hand, both experiment [1] and theory [2] have recently indicated that ferromagnetism may exist in crystals without transition metal ions.

We have analyzed the magnetic and the electronic structures of several II-V compounds. The calculations have been performed using the density functional theory and ultrasoft atomic pseudopotentials. Since II-V compounds crystallize in a variety of structures, it is important to determine the stable structure of the investigated systems. To this end we have considered 4 phases, namely the zinc blende, the rock salt, NiAs, as well as the $Zn_3P_2$ structure that is typical for several II-V crystals. In agreement with experiment, the most stable phase of SrN is the rock salt, which cohesive energy is lower than that of the $Zn_3P_2$ phase by about 0.2 eV/atom. Energies of both the zinc blende and the NiAs phases are considerably higher. Considering the magnetic properties we find that CaN, SrN, and BaN in the rock salt structure are spin polarized half-metals with the magnetic moment of 1 $\mu_B$ per unit cell. Analysis of their electronic structure demonstrates that the spin polarization originates in the spin polarization of isolated nitrogen atoms described by the Hund's rule. The polarization persists in solids due to their relatively large lattice constants and the high energy of the spin polarization of N. These results indicate that II-N compounds are magnetic materials with a new origin of spin polarization.

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[1] D. P. Young *et al*., Nature **397** (1999) 412.
[2] K. Kukasabe *et al*., J. Phys. C: Condens. Matter **16** (2004) 539.

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