Magnetism without magnetic ions: mixed valence monoclinic SrN

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Magnetic properties of solids result from the presence of transition metal or rare earth ions with partially filled *d* or *f* shells. Recently, a possible presence of ferromagnetism in systems without magnetic ions was considered. In particular, organic materials [1] as well as crystals containing high concentrations of native defects [2] were analyzed. Theory has also indicated the possibility of ferromagnetism in half-metallic II^A-V nitrides [3] (*e.g.*, CaN) in the metastable NaCl crystal structure. In the two latter cases, magnetism follows form the strong spin polarization of *p*(anion) orbitals.

Experimentally, the structure of SrN is monoclinic, *m*-SrN, with 16 atoms in the unit cell [4]. Nitrogen ions occupy two non-equivalent lattice sites. In the first one, an N ion is surrounded by Sr neighbors, while in the second one two neighboring N ions form a quasi-molecule N_2, characteristic also for the transition metal nitrides [5]. Consequently, one may expect that the charge states of the two types of N ions are different. This conjecture is supported by calculations of the electronic and magnetic structure based on the density functional theory. We find that *m*-SrN is indeed a mixed-valence crystal. A comprehensive analysis of the results show that (i) *m*-SrN is a metal with strong, almost half-metallic spin polarization at the Fermi level, (ii) magnetic moment of isolated N^{3-} ions vanishes, (iii) molecules N_2 are in the $\tilde{2}$ charge state and have a magnetic moment close to 1 μ_B. The obtained results point out to the presence of a ferromagnetic phase at low temperatures.

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