Possible pathways to new classes of ferromagnetic and half-metallic ferromagnetic materials

G.A.Sawatzky

University of British Columbia

I will discuss some ideas supported by theoretical calculations and some very recent experimental results that point to possible new classes of magnetic and halfmetallic ferromagnetic materials. All these ideas are based on defect structures in simple and also correlated oxides as well as substitution for O. Using model Hamiltonian and ab-initio band structure calculations we demonstrated that even large band gap nonmagnetic materials as simple as CaO can exhibit extraordinary properties like half-metallic ferromagnetism upon introducing a small concentration of Ca (not O !!) vacancies. The charge compensating holes in the O 2p band form states weakly bound to in the neighbouring shell of the Ca vacancy and these two hole states have a triplet ground state for finite and large Hubbard U's on Oxygen. This stabilization of the triplet state is due to a purely kinetic energy effect, the particular symmetry of the octahedron formed by the neighbouring ins and the difference in the symmetry for hole exchange for the triplet state and the singlet state. These so produced internal " molecules" quite generally have an effective strong Hund's rule coupling of the above kind but triplet ground states exist only for holes and not electrons. I will also discuss another theoretical and experimental study of the influence of N substitution providing evidence again of impurity states with a local moment and with ferromagnetic coupling. Recent photoemission and x ray absorption measurements on very thin films of SrO (N) confirm much of the theoretical predictions although ferromagnetism has not yet been observed. The basic Physics is somewhat different from that of a cation vacancy in that here use is made of the very narrow bands and the very strong atomic Hunds rule coupling of N as well as O.

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