### m46.001

# Crystal-chemistry design of new single-phase multiferroics

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Most single-phase multiferroics are of perovskite (or narrowly related) crystal structure. N. Hill pointed out the significant drawback of this kind of materials for multiferroism: as ferromagnetism (requiring "d<sup>n</sup>" configuration) and ferroelectricity (favoured by "d<sup>0</sup>" configuration) rely on the same cationic sublattice, this one should contain both "d<sup>n</sup>" and "d<sup>0</sup>" cations. This condition is hardly fulfillable and most of the multiferroic materials currently studied are derived from magnetic materials and do not contain "ferroelectrically active" cations such as  $Ti^{4+}$ , Nb<sup>5+</sup>, Ta<sup>5+</sup> ...

Our crystal-chemistry driven approach is to elaborate potentially multiferroic materials from ferroelectrics in which we may substitute magnetic cations without significant alteration of the "ferroelectric framework". Ferroelectrics possessing several cationic sublattices are the most likely candidates, and in the wide range of ferroelectric materials studied at the ICMCB, Tetragonal Tungsten Bronzes (TTB) appear to be the ideal ones.

We will present the structural, dielectric and magnetic properties of substituted TTB niobates, the multiferroic properties of which will be discussed in terms of crystal-chemistry. A survey of the "core-shell multiferroic composites" activities at the ICMCB will be also given.

### m46.o02

### **Complex Structure and Magnetism in Perovskite Multiferroics**

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Control of the spontaneous ferroelectric polarization (Ps) with an external magnetic field (H) in a material opens the opportunity for new types of magneto-electric devices. The realization of such devices is based on multi- ferroic materials in which magnetism and ferroelectricity are strongly coupled. While available multiferroics are limited, it has been shown that frustrated spin manganite perovskites may offer a new class of enhanced multiferroics [1-3]. In these manganites RMnO<sub>3</sub> (R=Gd,Tb,Dy), we find that multi-ferroic behavior arises as a consequence of the release of frustration with H. Here ferroelectricity arises below the N'eel temperature (TN), from a coupling to the lattice of an incommensurate (IC) modulation of the magnetic structure that is caused from frustration in the ordering of the Mn d orbitals [1, 3]. It is suggested the magnetic structure is spiral and breaks both time-reversal and inversion symmetry.[4] In this talk we will show that in TbMnO<sub>3</sub> magnetic field releases this frustration driving a magneto-structural transition from the IC phase with P parallel to the *c*-axis (P[|c]) to a commensurate phase with P[|a]. Using the magnetic structure at high field and the orbital ordering observed in TbMnO<sub>2</sub> at higher temperatures, the application of simple rules of super-exchange leads to a model that predicts the correct polarization for the high field phase in terms of the ordering of Mn-O-Mn bond angles.[5] This wark was done in collaboration with N. Aliouane, O. Prokhnenko and S. Landsgessel.

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