Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Interatomic spin-orbit coupling: mechanism for spin-spiral-caused ferroelectricity T.A. KAPLAN, S.D. MAHANTI, Michigan State University — There are two general classes of mechanisms that have been proposed for spin-spiral caused ferroelectricity, one based on ionic displacements as primary cause, the other on charge distortion without ionic displacements. Here we discuss the latter[1,2]. The mechanism proposed here is illustrated by a model where a pair of ions a and b each have low-lying s- and excited p- states with a prescribed spin state χ_a for the a-site states, similarly for the b-site, and there are 2 electrons; interatomic spin orbit coupling resides in inter-ion hopping due to s-p matrix elements of the spin-orbit coupling operator $\propto \nabla V \times \mathbf{p} \cdot \mathbf{s}$, $V, \mathbf{p}, \mathbf{s}$ are 1- electron potential, momentum, spin, respectively. Assuming the symmetry of a nearest-neighbor pair of cubic- spinel B-sites (there's no center of inversion (coi)) we find an electric dipole moment in the direction $\mathbf{r_{ab}} \times (\mathbf{S_a} \times \mathbf{S_b})$, as was found when there is a coi[1,2]. For the spins in a chain parallel to the spiral wave vector in $CoCr_2O_4$, direction [110][3], this results in ferroelectricity, as observed[4]; the spins in a [1,-1,0]-directed chain, give an antiferroelectric component. Extension to a pair of Cr^{3+} ions will be discussed.

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Date submitted: 14 Nov 2006 Electronic form version 1.4