

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

Sorting Category: 09.2 (T)

**Multiferroicity in half-doped manganites** SANJEEV KUMAR, Leiden University, GIANLUCA GIOVANNETTI, JEROEN VAN DEN BRINK, SILVIA PICOZZI — Using a joint approach of density functional theory and model calculations, we focus on unconventional physical mechanisms leading to multiferroicity in a prototypical half-doped manganite,  $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ . We focus on the strong competition between two exotic charge-orbital-spin ordered states. These are, (1) the charge and orbital ordered zig-zag spin state, also known as the CE-state, and (2) a spin-dimer Zener-polaron state. Both these states respect the inversion symmetry of the lattice and hence can not be ferroelectric. We identify a single variational parameter in terms of the coherent rotation of spin-dimers which interpolates between these two ordered states. It is shown that the true groundstate could be intermediate between these two and can break the inversion symmetry of the lattice. Using DFT calculations we show that the groundstate is indeed ferroelectric with a polarization up to few  $\mu\text{C}/\text{cm}^2$ .

Prefer Oral Session  
 Prefer Poster Session

Sanjeev Kumar  
kumar@lorentz.leidenuniv.nl  
Leiden University

Date submitted: 21 Nov 2008

Electronic form version 1.4