Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Sorting Category: 07.1.1 (E)

Electronic and Structural Properties Near the Ferroelectric Transition in Multiferroic Hexagonal $RMnO_3$ HAIYAN CHEN, TREVOR TYSON, TAO WU, New Jersey Institute of Technology, JIANMING BAI, Oak Ridge National Laboratory, KEN AHN, New Jersey Institute of Technology, KUMI PANDYA, Brookhaven National Laboratory, S.B. KIM, SANG-WOOK CHEONG, Rutgers University — Combined local and long range structural measurements were conducted on $RMnO_3$ for temperatures extending significantly above the ferroelectric transition temperature, (T_{FE}). We find in hexagonal RMnO3 no large atomic (bond distance or thermal factors) or electronic structure changes on crossing T_{FE}. The born effective charge tensor is found to be highly anisotropic at the O sites indicating very strong hybridization of the charge. The tensor does not change significantly above T_{FE} revealing no charge redistribution and suggests an unusual transition. Molecular dynamic simulations on large supercells are used to provide a general picture of the transition. This work is supported by DOE Grants DE-FG02-07ER46402 (NJIT) and DE-FG02-07ER46382 (Rutgers University).

[X] Prefer Oral Session
[ ] Prefer Poster Session

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Date submitted: 29 Dec 2011 Electronic form version 1.4