Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Effect of Pressure on the Atomic and Electronic Structure of Hexagonal $YMnO_3$.[1] ZHIQIANG CHEN, TREVOR TYSON, New Jersey Institute of Technology, SUNGBAEK KIM, SANG-WOOK CHEONG, Rutgers University — The multiferroic hexagonal system $YMnO_3$ is known to possess a significant polarization at room temperature. To understand the mechanism behind the polarization, we conducted high pressure x-ray diffraction measurements for pressures between ambient and 20 GPa. The powder diffraction data were refined to obtain the atomic level structure as a function of pressure. The pressure dependence of resistivity at room temperature (for pressures up to $\sim$6 GPa) was determined. Complementary density functional calculations were conducted to correlate the changes in electronic structure and polarization with the observed changes in atomic structure with pressure.

[1]This work is supported by DOE Grant DE-FG02-07ER46402.

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Date submitted: 27 Nov 2007 Electronic form version 1.4