Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Mode Coupling between the Nonpolar K_3 and Polar Γ_2^- Phonons as the Ferroelectricity Origin of Multiferroic h-$LuMnO_3$ SEUNGWOO SONG, SEUNGYANG HEO, HYUN MYUNG JANG, Division of Advanced Materials Science (AMS) and Department of Materials Science and Engineering, Pohang Univ of Sci & Tech — $LuMnO_3$ is expected to show the highest stability towards the hexagonal phase among 15 different lanthanide-based manganites. Currently, the most puzzling problem associated with the hexagonal $LuMnO_3$ (h-LMO) is the observed large temperature-gap between the structural phase transition to the polar $P6_3cm$ phase at $\sim$ 1290 K and the emergence of the spontaneous polarization at a substantially reduced temperature, $\sim$ 750 K. This anomalous temperature-gap has also been observed in h-$YMnO_3$. To resolve this puzzling issue, we have carried out density-functional theory calculations and found that the structural phase transition to the polar $P6_3$ cm phase from the nonpolar P63/mmc phase is mediated by the freezing-in of the zone-boundary K_3 phonon in h-LMO. However, the spontaneous ferroelectric polarization does not appear until the amplitude of K_3 phonon becomes a certain critical value above which the coupling of the polar Γ_2^- mode with the nonpolar K_3 mode is practically turned on. This mode-coupling-induced polarization, thus, elucidates the above puzzle.

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Date submitted: 11 Nov 2013 Electronic form version 1.4