Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structure and lattice distortion in $\mathbf{PbMg_{1/3}Nb_{2/3}O_3}$
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We investigated the local structural distortions of PMN($PbMg_{1/3}Nb_{2/3}O_3$) within the density functional theory using the linearized augmented plane-wave method. Structural relaxations were performed on 30 atom unit cells with B-cations arranged in 1:1 chemical ordering along [111]. The direction and magnitude of Mg and Nb off-centering within O_6 octahedral cages and Pb within its cage as well as electronic structures were examined. The results are discussed in terms of the Nb 4d - O 2p and Pb 6p - O 2p hybridizations and their interplay. A significant role is found for the on-site Ewald potential of different Nb sublattices, which is correlated with the off-centering.

†This work was supported by ONR and DOE.

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Date submitted: 21 Nov 2005 Electronic form version 1.4