Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ab Initio Investigation of Free Energy Landscape near Morphotropic Phase Boundary DUCHAO LV, Department of Materials Science and Engineering, The Ohio State University, JU LI, Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, YUNZHI WANG, Department of Materials Science and Engineering, The Ohio State University, XIAOBING REN, Ferroic Physics Group, National Institute for Materials Science, FRONTIER INSTITUTE OF SCIENCE AND TECHNOLOGY TEAM[1] — For pressure induced morphotropic phase boundary (MPB) in PbTiO3, although ground states have been investigated intensely, the overall free energy landscapes and so the transition paths are never systemically considered by ab initio method. Also there is little information about the oxygen octahedral tilts in monoclinic (M), orthorhombic (O) and triclinic (Tri) structures. In this work, in order to obtain the free energy landscapes, necessary oxygen octahedral tilts are considered not only in tetragonal (T) and rhombohedral (R) but also in M, O and Tri. According to the landscapes in the vicinity of MPB, firstly, the T-R transition path is not unique, since T-R and T-O-R paths have similar barriers; secondly, T-R barrier is ultra-low. Those explain the easy polarization rotation and so the ultra-high piezoelectric constant. Also, ground states are obtained by considering the oxygen octahedral tilts in T, R, M and O, and our results consist with the conclusion by J. Frantti, et.al in 2007. The fully relaxed M is actually T or R, which is indicated by the free energy landscapes. The ground state goes directly from T to R through MPB.

[1]in Xi'an Jiaotong University, China

Duchao Lv
Dept of Materials Science and Engineering, The Ohio State University

Date submitted: 26 Nov 2011 Electronic form version 1.4