Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

A route to high polarization multiferroics PRIYA MAHADEVAN, HIRAK CHANDRA, KAPIL GUPTA, ASHIS NANDY, S.N.Bose National Centre for Basic Sciences — Large ferroelectric polarizations are usually seen in d^0 ferroelectrics, while those with a finite d-electron count usually have a polarization which is two orders of magnitude smaller. The route then to high polarization multiferroics, seems quite obvious - examine if we can stabilize the d^0 type distortions in finite d-electron systems. The way we went about this was to dope carriers into $BaTiO_3$ and examine if ferroelectricity survived. Considering the example of V doping in $BaTiO_3$, we found that ferroelectricity was strongly stabilized, much stronger that in the undoped limit. Microscopic modeling coupled with ab-initio calculations revealed that part of the stability of the ferroelectric distortions about the V site emerged from first-order Jahn-Teller effects. The dilute doping limit was used to identify some design principles and helped us to design new multiferroics.

Priya Mahadevan
S.N.Bose National Centre for Basic Sciences

Date submitted: 08 Nov 2012 Electronic form version 1.4