Anomalous properties in ferroelectrics induced by atomic ordering[1]

A.M. George, Jorge Íñiguez[2] and L. Bellaiche

Physics Department,

University of Arkansas, Fayetteville, Arkansas 72701, USA; amgeorg@uark.edu

A first-principles derived approach is used to study *finite-temperature* properties of ordered and disordered $Pb(Sc,Nb)O_3$ ferroelectric alloys. We report unusual structural phases and huge electromechanical responses for certain atomic arrangements. Our $ab-initio$ simulations also reveal the microscopic mechanism responsible for these anomalies.

[1] Supported by Office of Naval Research (Grants N00014-01-1-0365, N00014-00-1-0542 and N00014-01-1-0600), the National Science Foundation (Grant DMR-9983678), and Arkansas Science and Technology Authority (Grant N99-B-21).

[2] Present address: Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA.