

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Reversible electro-strain coupling in K-doped BaTiO<sub>3</sub>**<sup>1</sup> SHI LIU, Geophysical Laboratory, Carnegie Institution of Washington, RONALD E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington and Department für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität — Ferroelectric materials that possess a spontaneous polarization have a wide range of applications. Coupled with a non-180° polarization switching, the strain of a ferroelectric crystal will change, due to the exchange of nonequal crystallographic axes. The field-induced large electro-strain coupling accompanied by non-180° domain switching, however, is usually an one-time effect, because the system lacks the driving force to recover to its original state, thus limiting its usefulness. It is suggested that defect dipoles introduced by dopant-vacancy pairs could serve as the driving force for reversible domain switching. However, there is still a lack of first-principles-supported microscopic understanding of the role of defect dipoles in reversible domain switching. In this work, we explore the intrinsic effects of K-dopants and oxygen vacancy on the 90° polarization switching in the prototypical ferroelectric BaTiO<sub>3</sub> with density functional theory. The interplay between polar defect dipole, vacancy concentration and electromechanical properties is investigated. We find that defect dipoles could drive the system back to its original state spontaneously after the electric field is turned off.

<sup>1</sup>S.L. is supported by Carnegie Institution for Science and R.E.C is supported by ONR.

Shi Liu  
Geophysical Laboratory, Carnegie Institution of Washington

Date submitted: 03 Nov 2015

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