# Stabilizing High Energy Piezoelectric Polymorphs

Lauren M. Garten[1*], Riley Whitehead[1], John Magnum[2], Shyam Dwaraknath[3], Laura Schelhas[4], Michael F. Toney[4], Julian Walker[5], Brian Gorman[2], Paul Ndione[1], Susan Trolier-McKinstry[5], Kristin Persson[3], and David Ginley[1]
[1]Material Science Center, National Renewable Energy Laboratory
15013 Denver West Parkway, Golden, CO, 80401
[2]Metallurgical & Materials Engineering, Colorado School of Mines,
1500 Illinois Street, Golden, CO 80401
[3]Materials Science and Engineering, University of California-Berkeley,
Hearst Mining Building, Berkeley, CA 94704
[4]SSRL Materials Science Division, SLAC National Accelerator Laboratory,
2575 Sand Hill Road, Menlo Park, CA 94025
[5]Materials Science and Engineering, The Pennsylvania State University,
Pollock Rd, State College, PA, 16802
*Lauren M. Garten: Lauren.garten@nrel.gov

Many technologically relevant materials are not at in a true thermodynamic minimum, but can still be stabilized under the right conditions. Recent work within the Materials Project has made over 1,000 first principle piezoelectric tensor calculations publicly accessible, many of which are for metastable materials.(*1*) From this list, two metastable materials, $SrHfO_3$ and $BaNiO_3$, present suitable candidates for lead-free piezoelectric alternatives. In both of these materials the challenge is in synthesizing the desired polymorph from a set of structures close in energy. This talk focuses on impact of stabilization techniques, such as epitaxial strain, heterostructural alloying, and kinetic trapping, on phase formation.

For the thin films of $SrHfO_3$ were deposited by pulsed laser deposition from an $SrHfO_3$ target onto single crystal Perovskite substrates. Deposition temperatures from 250-900 °C and partial pressure of oxygen from $10^{-1}$-$10^{-7}$ Torr were investigated. Deposition rate, and energy were also varied. Transmission electron microscopy in combination with selected area diffraction, synchrotron X-ray diffraction, and XRD pole figures suggest the formation of a P4mm piezoelectric structure that has not previously been reported.

Reference:

1. M. de Jong, W. Chen, H. Geerlings, M. Asta, K. A. Persson, A database to enable discovery and design of piezoelectric materials. *Scientific Data* **2**, 150053 (2015).