Strain-stabilizing new functionalities in BiMnO$_3$ and BiFeO$_3$

ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara, CLAUDE EDERER, Trinity College Dublin — Here we present first principles calculations of new functional phases of BiFeO$_3$ and BiMnO$_3$ stabilized by strain in thin film geometries. In BiFeO$_3$ we examine a supertetragonal-like phase recently identified in films grown on LaAlO$_3$ and YAlO$_3$ substrates.$^{1,2}$ We characterize the transition as a function of strain and find that it occurs between phases that are isosymmetric yet have dramatically different structures and properties, the most notable of which is a strong enhancement and rotation of the electric polarization.$^3$ From our computational results we suggest a model for the development of coexisting phases found in BiFeO$_3$ films on LaAlO$_3$ substrates.$^4$ In BiMnO$_3$ we demonstrate strain stabilization of an orbital ordering that gives rise to unusual ferroelectric and magnetic properties.

$^3$Hatt et al., arXiv:0909.4979.