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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.

[1]Béa *et al.*, Phys. Rev. Lett. **102**, 2009.
[2]Zeches *et al.*, Science **326**, 2009.
[3]Hatt *et al.*, arXiv:0909.4979.
[4]Zeches *et al.*, Science **326**, 2009.

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