

Abstract Submitted
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Tailoring the properties of 3d transition metal perovskite oxides through strain: a first-principles study OSWALDO DIÉGUEZ, Tel Aviv Univ, JORGE ÍÑIGUEZ, Luxembourg Institute of Science and Technology — In this talk I will present our recent computational work on how strain can stabilize phases that are higher-energy local minima of the bulk material of 3d transition metal perovskite oxides. Particular examples will include BiMnO_3 , that is a ferromagnet paraelectric in bulk, but we predict that it is a paramagnet ferroelectric as an epitaxial film, and $\text{Bi}_2\text{NiMnO}_6$, which we predict that is a ferroelectric ferromagnet when grown under epitaxial tension. We will also compare the behavior in bismuth transition-metal oxides with that in other perovskites such as BaTiO_3 and PbTiO_3 .

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