





The effect of strain in the properties of ferroelectric perovskite oxides: a first-principles study

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Abstract: In this talk I will present the recent work of our computational group regarding how strain can stabilize phases that are higher-energy local minima of the bulk material. Particular examples will include BiMnO₃, that is a ferromagnet paraelectric in bulk, but we predict that it is a paramagnet ferroelectric as an epitaxial film, and Bi₂NiMnO₆, 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 BaTiO₃ and PbTiO₃.