MAR15-2014-002219

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Complex-oxide multilayers by design: a treasure trove of unusual ferroic functionalities

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While inheriting most of the traits of their parents, layered variations of ABO_3 perovskites allow for a number of additional channels for property manipulation and fine-tuning. Their remarkable flexibility toward structural and chemical modification can be exploited for the design of new and advanced functionalities not originally present in the parent ABO_3 compounds. With the help of first-principles-based computational techniques, we have predicted intriguing electroactive behavior in layered-perovskite compounds of the Ruddlesden-Popper (RP) type. Specifically, we showed that Goldstone-like states (collective, close to zero frequency excitations, requiring practically no consumption of energy) can be induced in a $PbSr_2Ti_2O_7$ RP superlattice, manifesting themselves as easy rotations of the in-plane polarization vector. Examination of a fictitious epitaxial Ba_2TiO_4 RP compound demonstrated that it exhibits an assortment of competing incommensurate distortions, including ones that promote in-plane polarization. In this presentation we highlight the unusual behavior of a RP Ba_2ZrO_4 structure, which has already been synthesized as a bulk ceramic. An investigation of the properties of a (fictitious) epitaxial thin-film variant of this material reveals that under compression it undergoes a transition into an incommensurate state, while under tension it shows hints of a Goldstone-like polar instability, which surprisingly occurs without the presence of a lone-pair active ions like Pb or Sn. In both cases, we observe anomalies in the planar static dielectric susceptibility of the system, with large dielectric response predicted for the phase displaying the Goldstone-like instability.