Abstract Submitted
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ABO3 perovskite topological insulators: the enabling electronic motif and its structural stability[1] XIUWEN ZHANG[2], LEONARDO ABDALLA, QIHANG LIU, ALEX ZUNGER, RASEI, University of Colorado, Boulder, Colorado, United States — Oxide topological insulators (TI's) that could bring together the traditional oxide functionalities with the band topology of TI's have been sought for years. Here, we identify the electronic and structural motif ('topological gene') that achieves a topological band inversion in oxide perovskite as being a lone-pair B atom at the octahedral site in the cubic ABO3. However, at ambient pressure, the crystal structures that harbor the topological gene tend to develop an energy lowering distortion that removes the topological band inversion. We use this understanding to identify the 'window of opportunity' where TI-ness and stability can coexist: at moderate pressures the TI phases can be stabilized, bringing the 'topological gene' into coincidence with the 'stability gene'. This illustrates the fact that TI-ness and stability are sometimes contraindicated, and traces the approach that will be needed to establish their coexistence, tunable by external pressure.

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