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Tuning the structure of oxide thin films with strain ELIZABETH NOWADNICK, ANDREW MULDER, CRAIG FENNIE, Cornell University — Octahedral rotations are ubiquitous in perovskite oxides and play an important role in determining the functionality of these materials, for example impacting magnetism and ferroelectricity. Pressure applied to bulk perovskites, as well as biaxial strain in epitaxially grown thin films, couples to the octahedral rotations. By performing first principles density functional theory calculations for a wide variety of ABO_3 perovskite oxides, we present a systematic study of the structural response of these systems to pressure and strain. We find that the octahedral rotations respond to pressure and biaxial strain in distinct ways. With pressure, the relative compressibilities of the AO_{12} and BO_6 polyhedra govern the response of the octahedral rotations, whereas the response to biaxial strain arises from an interplay of the out of plane axis relaxation and the polyhedral compressibilities. Our findings offer insight into how to optimize the sensitivity of octahedral rotations to strain and pressure.

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