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**Coupling and competition between ferroelectricity, magnetism, strain and oxygen vacancies in  $AMnO_3$  perovskites** ASTRID MARTHINSEN, SVERRE MAGNUS SELBACH, Norwegian Univ Tech (NTNU) — First-principles calculations based on density functional theory is employed to investigate the interplay between oxygen vacancies, *A*-site cation size, epitaxial strain in the 001 plane, ferroelectricity and magnetism in the perovskite manganite series,  $AMnO_3$  ( $A = Ca^{2+}, Sr^{2+}, Ba^{2+}$ ). Increasing the unit cell volume through either chemical pressure or tensile strain generally lowers the formation energy of neutral oxygen vacancies. Increased volume also favors polar distortions, both because competing rotations of the oxygen octahedra are suppressed and because Coulomb repulsion associated with cation off-centering is reduced. Ferroelectric polarization favors ferromagnetism over antiferromagnetism as the polar distortion bends the Mn-O-Mn bond angles away from the optimal  $180^\circ$ . Polar distortions compete with the formation of oxygen vacancies, which have a higher formation energy in the polar phases; conversely the presence of oxygen vacancies suppresses the onset of polarization. In contrast, oxygen vacancy formation energies are lower for ferromagnetic than antiferromagnetic order. Our findings suggest a rich and complex phase diagram, in which defect chemistry, polarization, structure and magnetism can be modified using  $pO_2$ , strain, and electric or magnetic fields.

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