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Interplay of strain and oxygen vacancies in $CaMnO_3$ ULRICH ASCHAUER, RETO PFENNINGER, Materials Theory, ETH Zürich, SVERRE M. SELBACH, TOR GRANDE, Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, NICOLA A. SPALDIN, Materials Theory, ETH Zürich — Application of strain through heteroepitaxy has become an established route to engineering novel material properties such as multiferroism in perovskites. First principles calculations have been shown to accurately describe material properties as the in-plane lattice constants are changed by strain, and often indicate that large strain magnitudes (>4%) are required to induce new functionalities. At such large values, however, it is unclear whether strain will be accommodated primarily by changes in intrinsic lattice constants as usually assumed, or by the formation of point defects. Conversely, the use of strain to engineer point-defect concentrations and stoichiometry is largely unexplored. Here we use first-principles calculations to investigate the stability of the *Pnma* perovskite $CaMnO_3$ under bi-axial strain towards the formation of oxygen vacancies. We discuss the underlying mechanism for strain-vacancy coupling as well as the implications of our results for the growth of highly strained epitaxial films.

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