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Strain induced defects and charge state transitions in oxides

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It recently became apparent that bi-axial strain in coherent epitaxial perovskite oxide thin films or heterostructures can not only be accommodated by changes in structural parameters such as bond lengths or octahedral-rotation angles, but also by the formation of point defects. The redox reactions accompanying the formation of anion and cation vacancy defects lead to local volume changes, which facilitate the formation of either defect species under bi-axial strain. In this talk we will, after a general introduction to the phenomenon, use density functional theory (DFT) calculations to explore the generality of this concept for perovskite oxides and binary rock-salt oxides and put an emphasis on defects in different charge states. Moreover we will discuss the interaction of defects with ferroelectric domain walls, leading to novel functionalities in strained thin films.