

# Strain-defect interaction in oxides

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It recently became apparent that epitaxial strain in perovskite 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<sup>1,2</sup>. In this talk we will, after a general introduction, explore the generality of this concept for perovskite oxides of different compositions and with different functionalities as well as in binary rock-salt oxides. Based on our density functional theory calculations of the strained materials, the resulting point-defect-induced changes in properties such as the ionic and electronic conductivity, ferroelectricity and magnetism will be discussed.

1. Biškup, N. *et al.* Insulating Ferromagnetic LaCoO<sub>3</sub>- $\delta$  Films: A Phase Induced by Ordering of Oxygen Vacancies. *Phys. Rev. Lett.* **112**, 087202 (2014).
2. Aschauer, U., Pfenninger, R., Selbach, S. M., Grande, T. & Spaldin, N. A. Strain-controlled oxygen vacancy formation and ordering in CaMnO<sub>3</sub>. *Phys. Rev. B* **88**, 054111 (2013).