

Strain-defect interaction in oxides

Ulrich Aschauer, Materials Theory, ETH Zürich

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^{1,2}. 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 LaCoO₃- δ 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 CaMnO₃. *Phys. Rev. B* **88**, 054111 (2013).