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Probing functional perovskites through scanning transmission electron microscopy and first-principles theory[1]

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The aberration-corrected scanning transmission electron microscope (STEM) can provide real space imaging and spectroscopy at atomic resolution with a new level of sensitivity to structure, bonding, elemental valence and even spin state. Coupled with first-principles theory, this represents an unprecedented opportunity to probe the functionality of complex nanoscale systems. A number of examples will be shown, including the microscopic origin of the barrier to O vacancy transport across grain boundaries in Y-stabilized ZrO_2, the strain stabilized generation of a spin state superlattice in $La_{0.5}Sr_{0.5}CoO_{3-x}$ (LSCO) [1], the unexpected ferromagnetism in ultrathin, insulating $LaCoO_{3-x}$ (LCO) films [2] due to a vacancy superlattice (Fig. 1), and finally, the origin of the 2D electron gas at a $LaAlO_3/SrTiO_3$ interface is shown to be not due to vacancies but to the polar nature of the substrate [3].

Work performed in collaboration with J. Gazquez, N. Biškup, J. Salafranca, C. Cantoni, M. Varela and S. T. Pantelides.

[1] J. Gazquez, et al., Nano Lett, **11**, 973 (2011).
[2] N. Biškup, et al., Phys. Rev. Lett. **112**, 087202 (2014).
[3] C. Cantoni, et al., Adv. Mater. **24**, 3952 (2012).

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