

# Defects and defect-controlled behavior in oxide materials

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Atomic defects have an overriding effect on physical and chemical properties of oxide materials, and many technologies rely on detailed control of atomic impurities, promoters, or dopants, such as in gate oxides, optics, or (photo)catalysts of electronic states pinned at defects. Scanning probe microscopy (SPM) techniques allow characterization of these defects at the atomic scale, but interpretation remains challenging, particularly when only one signal is measured. In this work, we show how a combination of SPM and other experimental techniques with detailed Density Functional Theory (DFT) simulations can provide atomic scale characterization of defects and defect processes in two very different oxides.

As a demonstration of the approach, we use an interplay between simultaneously recorded non-contact atomic force microscopy (AFM) and scanning tunneling microscopy (STM) images [1] and DFT simulations, to reveal the location of single hydrogen species in the surface and subsurface layers of rutile TiO<sub>2</sub>. Subsurface hydrogen atoms are found to reside in a stable interstitial site as subsurface OH groups detectable in scanning tunneling microscopy as a characteristic electronic state, but imperceptible to atomic force microscopy [2].

For the insulating ternary metal oxide MgAl<sub>2</sub>O<sub>4</sub> (spinel), we combine NC-AFM, Surface X-ray Diffraction (SXRD) experiments and DFT calculations to reveal the detailed atomic-scale structure of the polar (100) surface [3]. Contrary to earlier predictions, the surface is terminated by an Al and O-rich structure with a thermodynamically favored amount of Mg-Al antisite defects. These are low-density defects in the bulk of MgAl<sub>2</sub>O<sub>4</sub>, but become a thermodynamically stable and integral part of the surface.

## References

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3. M. Rasmussen *et al.*, Phys. Rev. Lett. **107**, (2011) 036102