Graz Advanced School of Science
PHYSICS COLLOQUIUM OF THE UNIVERSITY OF GRAZ AND
THE GRAZ UNIVERSITY OF TECHNOLOGY

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From defect luminescence to cationic mixing: Oxide materials in the STM

Abstract:

Oxide materials are omnipresent in science and technology. Given their low carrier density and poor screening ability, oxide properties are often inhomogeneous in space and governed by stoichiometry modulations, defects and impurities. Spatially resolving techniques are therefore highly desired to probe the response of oxides in real space, best at the atomic length scale. In this talk, I will present two case studies, in which oxide surfaces have been investigated with scanning tunneling microscopy (STM) and embedded spectroscopic techniques.

The first study deals with cuprous oxide, one of the few p-type binary oxides. Cu_2O is known for its rich optical response, governed by para- and ortho-excitons and their unique trapping behavior at Cu and O defects. The material is thus ideally suited to be explored with STM conductance and luminescence spectroscopy at the nanoscale. For this purpose, thin-film and bulk $Cu_2O(111)$ surfaces were prepared and examined with respect to their morphology, electronic structure and local optical response. Both systems develop the characteristic nano-pyramidal reconstruction, and exhibit robust p-type conductivity with a 2.1 eV band gap. In classical photoluminescence, free and defect-bound excitons are detected for the bulk crystal, while only emission from single and double charged O vacancies is found for thin films. In STM luminescence, Cu-vacancy emission and a remnant of the free-exciton peak is detected on bulk crystals. Corresponding photon maps of the surface are highly homogenous due to long exciton diffusion lengths that destroy any correlation between the excitation and decay point of the optical modes. Conversely, Cu_2O films exhibit a broad emission band between 700-950 nm that is compatible with cavity plasmons stimulated by inelastic electron tunneling. Moreover, resonant tunneling into V_O gap states gives rise to highly localized photon emission that can be associated to single O vacancies in the surface.

In the second part, the formation of ternary oxides is discussed, as realized by mixing Fe and V atoms in a reactive ambience on Pt(111) and Ru(0001) supports. Atomically resolved STM measurements enable us to locate the different cations in the oxide surface, providing unmatched insights into their mixing characteristics. With the help of DFT calculations, we find that formation of Fe-V mixed pairs is energetically favored, while Fe-Fe pairs have strongly repulsive character. Monte Carlo simulations based on effective interaction energies perfectly reproduce the Fe/V distribution found in the experimental data. Surprisingly, while Fe/V mixed oxide films on Pt(111) develop in a wide composition range, only a 1:1 stoichiometry between Fe and V can be stabilized in mixed oxides on Ru(0001). The observation can be rationalized with site-selective binding properties imposed by an oxygen interface layer that develops on the Ru but not on the Pt substrate.

In summary, my talk demonstrates how STM techniques can be exploited to unravel the diversity of oxide properties at the nanoscale, despite the insulating nature of many bulk oxides.

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Host: Martin Sterrer

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