# New Trends in Structural Electronic Characterization of Materials, Interfaces, and Surfaces Using Synchrotron and FEL Based Light Sources Focus Topic

## Room On Demand - Session LS-Contributed On Demand

## New Trends in Structural Electronic Characterization of Materials, Interfaces, and Surfaces Using Synchrotron and FEL Based Radiation Sources Contributed On Demand Session

**LS-Contributed On Demand-1 Resolving Interfacial Electronic Structure in Thin Film Heterostructures using Resonant X-ray Reflectometry*, Ryan Need,*** University of Florida

The interfaces between electronic materials are critically important for the operation of modern electronic devices and the pursuit of new knowledge in solid state physics. Today, the interest in electronic interfaces is fueled by emerging technologies like quantum computing, spintronics, and energy storage, along with fundamental questions about how tuning symmetry and band topology at interfaces can modify functional properties. Answering these questions requires the development of characterization probes that have high spatial and spectral resolution, a wide range of sample environments, and are compatible with in-situ or in-operando experiments.

In this talk, we argue that resonant X-ray reflectometry (RXR), which combines the element-specificity and local structure sensitivity of X-ray absorption spectroscopy with the Angstrom depth-resolution of reflectometry, is the probe best suited to this challenge. As an example, we show how RXR can be used to extract electronic structure depth profiles in complex oxide superlattices and visualize interfacial charge transfer with atomic layer resolution. Specifically, we present measurements collected from SmTiO$_3$(SmTO)/SrTiO$_3$ (STO) superlattices with STO quantum wells varying in thickness from five SrO planes to a single SrO plane. At the polar-nonpolar SmTO/STO interface, a known electrostatic discontinuity leads to approximately half an electron per areal unit cell transferred from the interfacial SmO layer into the neighboring STO quantum well. We observe this charge transfer as a suppression of the Ti t$_{2g}$ absorption peaks that minimizes contrast with the neighboring SmTO layers at those energies and leads to a pronounced absence of superlattice peaks in the reflectivity data. Critically, our results demonstrate the sensitivity of RXR to electronic reconstruction in the monolayer limit and prove RXR to be a powerful means of characterizing interfacial electronic structure in quantum materials.

**LS-Contributed On Demand-4 HAXPES Study of Surface/Interface Effects Induced by Heavy Alkali Post Deposition Treatment of (Ag,Cu)(In,Ga)se2 Thin Film Solar Cell Absorbers*, Natalia Martin,*** Uppsala University, Sweden*; T. Törndahl,* Uppsala University , Sweden*; K. Simonov,* Department of Materials and Process Development Swerim AB, Sweden*; H. Rensmo, C. Platzer-Björkman,* Uppsala University, Sweden

Solar cells based on Cu(In,Ga)Se$_2$ (CIGS) thin film absorbers have shown high and stable efficiencies for both laboratory cells and industrial modules with recent record cell efficiencies of 23.4% [1]. In order to reach closer to the theoretical maximum efficiency of around 30%, further reductions of optical and electrical losses are needed. Some recent works show that silver (Ag) alloying in CIGS to form (Ag,Cu)(In,Ga)Se$_2$ (ACIGS) leads to higher device efficiencies as compared to similar CIGS devices without Ag [2]. More, a postdeposition treatment (PDT) based on the alkali metal fluorides (i.e., KF, RbF or CsF) [3] after absorber formation has been studied recently and is known to improve the efficiency in CIGS solar cells, mainly by an increase in the open circuit voltage, V$_{OC}$. The exact role of the silver and/or alkali elements is intensively discussed, but it is clear that interface and grain boundary effects are important in (A)CIGS solar cells. It is likely that a redistribution of the absorber elements near the surface region may occur during the alkali PDT and some works show interface formation in CIGS solar cells subjected to a metal fluoride post deposition treatment [4].

In this work we employed hard X-ray photoelectron spectroscopy (HAXPES) to study the interface between CdS buffers and PDT-ACIGS absorbers, which have been exposed to different metal fluoride PDT. Two different alkali PDT are compared, RbF and CsF, to investigate how the choice of the metal fluoride treatment affects the buffer/absorber interface. In particular, the chemical and electronic properties of CdS/ACIGS interfaces in terms of intermixing, energy band alignment and composition for a set of device relevant samples have been studied.

The results show that the electronic structure at the CdS/ACIGS interface does not change for the different PDTs. However, the ACIGS composition at the near surface region seems to change depending on the applied PDT process. Possible reasons for this will be discussed. The results give insights into how selective alkali PDT could change the ACIGS surface composition, which may influence the solar cell behavior.

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**LS-Contributed On Demand-7 Surface Action Spectroscopy With Inert Gas Messenger Atoms*, Hans-Joachim Freund,*** Fritz Haber Institute of the Max Planck Society, Germany

Action spectroscopy is well established in the field of cluster physics and chemistry, where sample densities are very low. The action spectroscopy approach is based on the idea, that messenger species are attached to the object under investigation, and that laser light of varying frequency in the infrared is used to detach the messengers, which are detected with a mass-spectrometer. By varying the infrared frequency, one is able to record the vibrational spectrum of the object under study without having to record a reference spectrum. It has not been applied to surfaces due to the need for high intensity frequency variable laser sources. On the other hand, desorption induced by electronic transition as well as photo-desorption are well established fields surface science. We have over the last few years developed surface action spectroscopy employing the Free Electron Laser installed at the Fritz-Haber Institute. In the presentation I report on the conceptual design and some first results on surface vibrational spectroscopy using the approach (1-3), as well as the pros and cons of the techniques in comparison to other vibrational spectroscopy techniques.

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**LS-Contributed On Demand-13 X-ray Magnetic Linear Dichroism Studies of Electrical Switching of Antiferromagnetic Order in α-Fe2O3 Epitaxial Films*, Egecan Cogulu,*** *N. Statuto,* New York University*; Y. Cheng,* Department of Physics, Ohio State University*; S. Yu, F. Yang,* Ohio State University*; R. Chopdekar, H. Ohldag,* Advanced Light Source, Lawrence Berkeley National Laboratories*; A. Kent,* New York University

Recently manipulation of antiferromagnetic (AFM) order has been gaining the attention of the spintronics community. Magnetic switching has been reported in AFM thin films based on electronic transport methods, which provide only spatially averaged information on AFM states. Other techniques, such as x-ray magnetic linear dichroism (XMLD), can provide local information on AFM domains. In this study, we report direct observation of spin reorientation in response to current pulses in (0001) α-Fe$_2$O$_3$/Pt heterostructures. Our experiment combines the application of current pulses and spatially resolved photoemission electron microscopy (PEEM) with X-ray magnetic linear dichroism to detect antiferromagnetic contrast. Pulses were applied in two different configurations A and B (Fig. 1a), and XMLD images were interleaved with current pulse sequences to reveal changes in the AFM domains (Fig. 1c). Our analysis shows that electrical pulses do not only reorient the Néel vector within the easy plane as previous work indicates. Instead, we conclude that most of the change current induced change associated with the Néel vector is a rotation out of the film plane, and different pulse directions can bring the AFM order in and out of plane deterministically.

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**LS-Contributed On Demand-16 Probing Interfacial Ferromagnetism in Oxide Superlattices Using Depth Resolved X-Ray Spectroscopic and Scattering Techniques***, **Jay Paudel,*** Temple University*; M. Terilli,* Rutgers University*; I. Vobornik, P. Orgiani, G. Panaccione,* CNR-IOM, TASC Laboratory, Italy*; C. Klewe, P. Shafer,* Advanced Light Source, LBNL*; V. Strocov,* Swiss Light Source, PSI, Switzerland*; J. Chakhalian,* Rutgers University*; A. Gray,* Temple University

The origins of emergent interfacial ferromagnetism in $CaMnO_3/CaRuO_3$ and $CaMnO_3/LaNiO_3$ heterostructures have been investigated for nearly two decades [1-4]. Several experimental and theoretical studies suggest that this phenomenon is stabilized by charge transfer across the interface and suggest different thicknesses of the resultant ferromagnetic layers. In this comprehensive study, we have carried out polarization-dependent x-ray absorption spectroscopy and x-ray resonant magnetic scattering to probe the depth-resolved magnetic profile at the interfaces in these material systems. Furthermore, we have utilized bulk-sensitive hard x-ray photoemission spectroscopy and soft x-ray standing-wave photoemission spectroscopy in both first- and second-order Bragg geometries to probe the depth-dependent chemical profile and interfacial charge reconstruction in $CaMnO_3$. Finally, high-resolution angle-resolved photoemission spectroscopy with in-situ pulsed-laser deposition synthesis were used to track the topology of the Fermi surface of $LaNiO_3$ in the superlattice across the thickness-dependent metal-insulator transition. The results were compared to the first-principles theoretical calculations.

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