

SYNF 3: Ferroic materials and novel functionalities III - Poster (joined by O posters)

Time: Tuesday 18:30–19:30

Location: Poster F

SYNF 3.1 Tue 18:30 Poster F

La and Mn co-doping effects on the structure and electrical properties of BiFeO₃ thin films — ●ABDELILAH LAHMAR¹, GIRAY KARTOPU¹, SALAH HABOUTI¹, CLAUS-HENNING SOLTERBECK¹, MOHAMMED ES-SOUNI¹, BRAHIM ELOUADI², and MICHEL COUZI³ — ¹Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany — ²Université de La Rochelle, Department de Chimie, La Rochelle, France — ³Laboratoire de Physico-Chimie Moléculaire, CNRS, Université Bordeaux, Talence, France

The structural, electric, and magnetic properties of the solid solution Bi_{1-x}La_xFe_{1-x}Mn_xO₃ (0 ≤ x ≤ 0.1) have been investigated. Thin films have been grown by a sol-gel spin-coating method on (111)Pt/Ti/SiO₂/Si substrates. The incorporation of both (La³⁺, Mn³⁺) cations in bismuth ferrite host lattice was found to improve dielectric, ferroelectric, and magnetic properties. A comparative study of 5%La-, 5%Mn-, and 5%LaMn- doped BiFeO₃ has been undertaken with the aim of understanding the role of each doping element on the structure and electrical properties. Raman spectroscopy has been used for a detailed structural characterization, and the results obtained are compatible with our ferroelectric investigations.

SYNF 3.2 Tue 18:30 Poster F

HX-PES study of LaAlO₃/SrTiO₃ heterostructures — ●GÖTZ BERNER¹, ANDREAS MÜLLER¹, STEFAN THIEL², CHRISTOF SCHNEIDER², MICHAEL SING¹, JOCHEN MANNHART², and RALPH CLAESSEN¹ — ¹Experimentelle Physik IV, Universität Würzburg — ²Experimentelle Physik VI, Universität Augsburg

Oxide heterostructures are of special interest due to the unexpected new physics occurring at the interface. E.g., a quasi-two-dimensional electron gas (2DEG), which even becomes superconducting at low-

est temperatures forms at the interface of the two band insulators LaAlO₃/SrTiO₃, if at least 4 unit cells of LaAlO₃ are grown on TiO₂ terminated SrTiO₃.

In principle, angle dependent hard x-ray photoemission spectroscopy (HX-PES) is a powerful tool to get insight in both the change in chemical state and the vertical distribution of the additional charge at the interface by probing the intensity ratio of the Ti³⁺ 2p and Ti⁴⁺ 2p core lines. However, first measurements surprisingly did not show any Ti³⁺ 2p signal for various detection angles. This is in sharp contrast to the expectation from simple electrostatic considerations and recent estimates from SXRD measurements. Both claim an area carrier density corresponding to 0.5 electron per unit cell. In contrast, our HX-PES measurements indicate a much lower carrier concentration consistent with Hall measurements on our samples. As possible explanation for these discrepancies we discuss the effects of the finite LaAlO₃ thickness and the oxygen defects at the interface.

SYNF 3.3 Tue 18:30 Poster F

Hybrid-functional applied to a model ferroelectric: SrTiO₃ — ●ROMAN WAHL — University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

The structural, electronic and phonon properties of the cubic and tetragonal phase of SrTiO₃ are studied from *ab initio*. The calculations are performed in the pseudopotential DFT framework using the local density approximation (LDA), gradient corrected functionals (PBE, PBEsol) and hybrid functionals (HSE03) as implemented in the Vienna *ab initio* simulation package (VASP). Due to the large variation of theoretical predictions for the frequency of the *F*_{1u} (Γ₁₅) zone-center phonon mode (100i - 64 cm⁻¹) special attention is put on this particular mode and its volume dependency.