DF 16: Crystallography in Materials Science (KR with DF, MI)

Time: Thursday 15:40–17:00 Location: H26

DF 16.1 Thu 15:40 H26

Low temperature synthesis of $CuFeO_2$ (delafossite) between 50°C and 90°C: A new process solely by precipitation and ageing — •Melanie John[1], Aladin Ullrich[2], and Soraya Heuss-Assbichler[1] — [1]Ludwig-Maximilians-Universität München, München, Deutschland — [2]Universität Augsburg, Augsburg, Deutschland

Due to the large variability of technical applications of delafossite compounds e.g. as a catalyst, in p-type conduction oxides or as a cathode in Li-ion batteries, the synthesis of ABO_2 structures have received much attention the last years. Delafossite syntheses have been reported via solid state reaction and sol-gel processes using high temperatures between 900-1200°C or hydrothermal synthesis methods using at least autogenous pressure so far. We now synthesized $CuFeO_2$ nanoparticles, the parent mineral of the Delafossite group, solely by precipitation and subsequent ageing at temperatures between 50°C and 90°C and without any additives controlling the oxidation state of copper for the first time. With this method, it is possible to synthesize a mixture of 2H (space group (SG): $P6_3/mmc$) and 3R polytype (SG: R-3m) of delafossite showing hexagonal morphology within 10 hours. The experimental conditions regulate the phase assemblage, size and the necessary ageing time. The synthesized material was analyzed by ICP-OES, FTIR, XRD, SEM, TEM and magnetic measurements.

DF 16.2 Thu 16:00 H26

Investigation of the sodium solid electrolyte $Na_5YSi_4O_{12}$ — •Wolfram Münchgesang[1], Anastasia Vyalikh[1], Falk Meutzner[1], Tina Nestler[1], Dörte Wagner[2], Axel Rost[2], Ulrike Langklotz[2], Jochen Schilm[2], Tilmann Leisegang[1], and Dirk C. Meyer[1] — [1]Technische Universität Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg, Germany — [2]Fraunhofer Institute für Ceramic Technologies and Systems IKTS, Winterbergstraße 28, 01277 Dresden, Germany

Beside the well-known sodium solid electrolytes β-Alumina and NASICON, $Na_5YSi_4O_{12}$ (NYS) is another promising crystal structure with a high ionic conductivity. Its main advantage over the two abovementioned structures is the reduced production complexity and the associated costs. However, very little is known about its complex crystal structure and properties. Starting from a crystallographic point of view, sodium ion conduction pathways have been considered with the Voronoi-Dirichlet and the energy-scaled bond valence approaches, and compared with the pathways in other ion conductors.
In the present work, the crystal structure and ionic conductivity in polycrystalline NYS-materials, obtained by a glass-ceramic process, has been analysed using solid-state NMR and Electrical Impedance Spectroscopy respectively, and interpreted in respect to the theoretical predictions.
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DF 16.3 Thu 16:20 H26

Measuring electron-phonon coupling by RIXS: the showcase of anatase TiO2 — •Simon Moser[1], Sara Fatale[1], Peter Krüger[2], Helmuth Berger[1], Philippe Bugnon[1], Arnaud Magrez[1], Hideharu Niwa[3,4], Jun Miyawaki[3,4], Yoshihisa Harada[3,4], and Marco Grioni[1] — [1]Ecole Polytechnique Federale de Lausanne, Switzerland — [2]University of Chiba, Japan — [3]University of Tokyo, Japan — [4]SPring-8, Japan

Anatase TiO2 has been proposed for many applications from transparent conducting panels to photovoltaic- and photocatalytic- devices, as well as memristors. However, little is known about the dynamics of the doped-in charge carriers in this textbook insulator. Recently, we have shown by angle resolved photoemission (ARPES) that these populate the bottom of the conduction band and strongly couple to an optical phonon mode, forming so called large polarons (Moser et al., PRL 110, 196403, 2013).

In the present study, we take the point of view of the phonon. By means of bulk-sensitive resonant inelastic X-ray scattering (RIXS) at the Ti L3 edge. We find that the formation of the polaron cloud involves a single 95 meV phonon along the $c-$axis, besides the 108 meV ab-plane mode previously identified by ARPES. The coupling strength to both modes is the same within error bars, and it is unaffected by the carrier density. This establishes RIXS as a directional and bulk-sensitive probe of electron-phonon coupling in solids (Moser et al. PRL 115, 096404, 2015).

DF 16.4 Thu 16:40 H26

Polycrystalline organic semiconductors studies by X-ray nano diffraction — •Clemens Liewald[1,2], Simon Noever[1,2], Stefan Fischer[1], Janina Roemer[1], and Bert Nickel[1,2] — [1]Fakultät für Physik & Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München — [2]Nanosystems Initiative Munich, Schellingstrasse 4, 80799 München

The efficiency and reliability of organic semiconducting devices depends strongly on the knowledge of the nanoscale arrangement in the active organic layers. Here, we report on the possibilities of X-ray nanodiffraction to characterize polycrystalline organic thin films at beamline ID01, ESRF, before and after its upgrade. The beam diameter in our measurements is 110 nm at 8.9 keV and 350 nm at 20 keV. We find a high beam damage at 8.9 keV compared to only little damage at 20 keV. First, we apply the focused X-ray beam to a multilayer device, with different organic and inorganic layers, and demonstrate the possibility to measure buried microstructures in e.g. the active organic layer under and next to gold electrodes. Second, we explore the local distribution of two polymorphs in a single pentacene thin film. The lateral shape and distribution of these polymorphs can be mapped with infrared (IR) scanning near-field optical microscopy (SNOM) and is compared to the amplitude from the focused X-ray beam at ID01. In future, the combination of X-ray nanodiffraction with e.g. IR-SNOM as a correlated microscopy will allow to gain various new insights to the influence of the nanoscale crystallinity on the efficiency of organic electronics devices.