KFM 27: Postersession KFM

Time: Thursday 15:00–17:00 Location: Poster E

KFM 27.1 Thu 15:00 Poster E

Frequency shifts and Raman signatures at ferroelectric domain interfaces of $LiNbO_3$ and $LiTaO_3$ — Sergej Neufeld[1], Michael Rüsing[1], •Simone Sanna[2], Gerhard Berth[1], Artur Zrenner[1], and Wolf Gero Schmidt[1] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Justus-Liebig-Universität Giessen, Institut für Theoretische Physik, 35392 Gießen, Germany

Periodically poled lithium niobate ($LiNbO_3$, LN) and lithium tantalate ($LiTaO_3$, LT) structures are of particular technological interest as waveguides and SHG structures. The interface between neighboring domains features a large polarization gradient, which is accompanied by a modulation of numerous physical properties such as internal strain, birefringence and Raman cross section. In recent years, several experimental techniques, including Raman spectroscopy [1], have been utilized to image domain walls. In this work, vibrational properties and Raman signatures of LN and LT in the vicinity of domain walls are studied phenomenologically within an atomistic model via density functional theory calculations. Additionally, Raman signatures of LN and LT domain walls are studied experimentally via a confocal Raman setup. The frequency shifts and Raman intensities of E and A_1 modes calculated along a phenomenological reaction coordinate between both phases are in qualitative agreement with the measured data. In particular, the well-known soft mode behavior of the low frequency A_1-TO_1 mode is reproduced in the calculations.

[1] Appl. Phys. B 78, 363-366 (2004)

KFM 27.2 Thu 15:00 Poster E

Ferroelastic domain identification in $BiFeO_3$ crystals using Raman spectroscopy — •Jan Rix[1], Cameliu Himcinschi[1], Christian Röder[1], Martin Rudolph[2], Mingmin Yang[3], David Rafaja[2], Jens Kortus[1], and Marin Alexe[3] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Multiferroic $BiFeO_3$ crystals have been investigated by means of Raman spectroscopy using 442 nm (resonant conditions) and 633 nm (non-resonant conditions) laser wavelengths. The azimuthal angular dependence of the intensity of the Raman modes allowed an assignment to one of five symmetry characters, which are present in the directional dispersion [1,2]. Mixed symmetries were taken in account, considering the orientation of the optical c-axis along the pseudo-cubic $<111>_{pc}$ direction. The experimental data have been verified by a Raman tensor formalism simulation. The strong intensity variation of the polar Raman modes at 138 cm^{-1} ($\mathbf{E}_{TO}$ - $\mathbf{A}_{1TO}$) and at 172 cm^{-1} ($\mathbf{A}_{1LO}$ - $\mathbf{E}_{LO}$) were used for line scans, mappings and a depth profile in order to identify the elastic domain patterns. The distribution of domains found by Raman spectroscopy is in very good agreement with the domain pattern revealed by Electron Back Scattering Diffraction (EBSD) and Piezo-Force Microscopy (PFM).

[1] J. Hlinka et al. Phys. Rev. B 83, 020101 (2011). [2] A. Talkenberger et al. J. Raman Spectrosc. 46, 1245 (2015).

KFM 27.3 Thu 15:00 Poster E

Domain evolution in a Ba(Zr0.2Ti0.8)O3-0.5(Ba0.7Ca0.3)TiO3 piezoceramic studied by piezoresponse force microscopy — •Xijie Jiang, Na Liu, Robert Stark, and Christian Dietz — Technische Universität Darmstadt, Alarich-Weiss-Str. 16, Darmstadt, Germany

Lead-free (1-x)Ba(Zr0.2Ti0.8)O3-x(Ba0.7Ca0.3)TiO3 (BZT- xBCT) ceramics have drawn special attention to researchers because of their outstanding dielectric and electromechanical properties, competitive to lead zirconate titanate (PZT). In particular, BZT-0.5BCT was reported to have a piezoelectric coefficient of 620 pC/N explained by the existence of a triple point close to room temperature. However, the fundamental mechanisms behind the functionality of this ferroelectric are not completely understood. Here, we use piezoresponse force microscopy (PFM) to observe the domain evolution of a BZT-0.5BCT ceramic while changing the temperature and the applied voltage between tip and sample. In the initial state, the sample exhibits a combination of wedge-shaped and lamellar domains. During the increase of the applied voltage to +30 V, the observed area formed a single domain state. Subsequently decreasing the applied voltage step-wise to -30 V and increasing back to 0 V caused the sample to form wedge-shaped and lamellar domain again. Thus, the sample reversibly transforms from a multi-domain to a single-domain state during a complete poling cycle. During heating to 60 °C, most wedge-shaped domains transformed to lamellar domains and the orientation of the domain configuration was partially reversed.

KFM 27.4 Thu 15:00 Poster E

Towards a proof of water splitting via pyroelectrolysis — •Thomas Köhler, Wolfram Münchgesang, Erik Mehner, Juliane Hanzig, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany

The generation of hydrogen through water electrolysis has been understood for a long time and will be used for large-scale conversion of electrical energy into chemical energy in the future. The direct conversion of residual heat into hydrogen is completely new to our knowledge, but feasible when making use of pyroelectric materials. In pyroelectrolysis, a cyclic temperature excitation generates an electric field between the crystal surfaces due to an imbalance between polarization and compensation charges. For water electrolysis, this electric field must exceed the redox potential of water.

A pyroelectolysis cell was developed for investigating the interaction of congruent $LiTaO_3$ with aqueous media, in order to record the surface potential during the temperature change and the reaction rate of the pyroelectolysis. A sufficiently high voltage difference between the opposite crystal surfaces caused by cyclic temperature changes was observed. This satisfies the basic requirement for water splitting on the pyroelectric surface. Cyclic voltammetry of the electrolyte solution was applied for electrochemical detection of the water splitting reaction. To finally prove water splitting, the increasing educt concentration in the electrolyte solution would be monitored as a change of the oxidation and reduction peaks.

KFM 27.5 Thu 15:00 Poster E

Anisotropic Transport of the 2D Electron System in (001) Al_2O_{3-d}/SrTiO3 Heterostructures — •Karsten Wolff[1], Roland Schäfer[1], Richard Thelen[2], Matthias Meffert[3], Dagmar Gerthsen[3], Rudolf Schneider[1], and Dirk Fuchs[1] — [1]Karlsruher Institut für Technology, Institut für Festkörperphysik — [2]Karlsruher Institut für Technology, Institut für Mikrostrukturtechnik — [3]Karlsruher Institut für Technology, Laboratorium für Elektronenmikroskopie

Transport measurements on the two-dimensional electron system in $Al_2O_3/SrTiO_3$ heterostructures indicate significant non-crystalline anisotropic behavior below T ≈ 30 K. Lattice dislocations in $SrTiO_3$ and interfacial steps are suggested to be the main sources for electronic anisotropy in (001) oriented heterostructures. Anisotropic defect scattering likewise alters magnetoresistance at low temperature remarkably and influences spin-orbit coupling significantly by the Elliot-Yafet mechanism of spin relaxation resulting in anisotropic weak localization. Applying a magnetic field parallel to the interface results in an additional field-induced anisotropy of the magnetoconductance, which can be attributed to Rashba spin-orbit interaction.

KFM 27.6 Thu 15:00 Poster E

Investigation of magneto-ionic effects on Au-Fe (core-shell) nanowires — •Martin Nichterwitz[1,2], Shashank Honnali[1], Tom Sieger[1], Diana Pohl[1], Anna Niemann[1], Kornelius Nielsch[1], and Karin Leistner[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Technische Universität Dresden, Physikalische Chemie, 01062 Dresden, Germany

Miniaturization and the demand for low-power devices led to increasing research of voltage-controlled devices, which do not show effects like joule heating. It was recently shown that reversible magneto-ionic manipulation with up to 64 % change in magnetization of Fe/FeOx films is possible at room temperature in liquid alkaline electrolytes. [1,2] The change of geometry from thin films to nanowires (NW) promises enhanced magneto-ionic effects due to the higher surface/volume ratio. We present an approach to observe the above stated effect using Au-

Fe-NWs (core-shell). Au-NWs are grown by electrodeposition into a nano-porous Al2O3-template. Individual Au-NWs are electrically contacted on a glass substrate using laser lithography and a metallization process. Subsequently, a 5-10 nm thick Fe shell is electrodeposited on the Au-NW. To investigate the magneto-ionic effects, in-situ measurements (resistivity and magnetization) will be performed under different potentials in liquid alkaline electrolytes. This is expected to lead to the reversible switching between ferromagnetic and non-ferromagnetic states in the Fe/FeOx shell on the NW, due to reduction and oxidation processes, respectively. [1] K. Duschek et al., Electrochem. Comm. 72, 2016, 153 [2] K. Duschek et al., APL Mater. 4, 2016, 032301

KFM 27.7 Thu 15:00 Poster E

Interplay of oxygen vacancies and conductance in SrMnO3 thin films under epitaxial tensile strain — Lokamani Lokamani[1], Carina Faber[3], Peter Zahn[1], Nicola Spaldin[3], and •Sibylle Gemming[1,2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — [3]Materials Theory, ETH, 8093 Zürich, Switzerland

Strontium manganate (SrMnO3), a perovskite polymorph, exhibits cubic structure at low temperatures, which transforms under tensile strain into a G-type-antiferromagnetic (G-AFM) antiferrodistortive polar phase in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in 20nm thin films of SrMnO3 under 1.7% tensile strain on (001)-oriented LSAT grown in an oxygen-deficient atmosphere[2]. Strikingly, the individual domains show different conductance features, whereas the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitors with high charge rention times.

Here, we present a detailed first-principle investigation of the domain wall formation in strained SrMnO3, their electronic properties and the influence of oxygen vacancies on the 2D-electron gas at the polar domain walls. Preliminary results on the migration energetics of the oxygen vacancies are expected.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)
Funding by VI Memriox(VH-VI-422) & Nanonet(VH-KO-606)

KFM 27.8 Thu 15:00 Poster E

Direct measurements of electrocaloric effect in Barium Titanate single crystals — •Maksim O. Karabasov, Mehmet Sanlialp, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany

The electrocaloric effect (ECE) is studied for barium titanate single crystals utilizing two direct measurement methods. The adiabatic electrocaloric temperature change is observed by applying an electric field to the barium titanate single crystals in a quasi-adiabatic calorimeter. The second method uses the enthalpy change in a modified differential scanning calorimeter (DSC) to calculate the electrocaloric temperature change [1]. The focus of this study is to examine the anisotropy of ECE by applying electric fields for [001], [011] and [111] oriented single crystals. The anisotropy of the ECE leads to a possible negative temperature change, i.e. a temperature decrease by application of an electric field during the orthorhombic-tetragonal phase transition of Barium Titanate, if the field orientation favors the higher temperature/entropy phase [2].

[1] M. Sanlialp et al., Appl. Phys. Lett. **111**, 173903 (2017)
[2] M. Marathe et al., Phys. Rev. B **96**, 014102 (2017)

KFM 27.9 Thu 15:00 Poster E

Polaron optical absorption in congruent lithium niobate from time-dependent density-functional theory — •Michael Friedrich[1], W. G. Schmidt[1], Arno Schindlmayr[1], and Simone Sanna[2] — [1]Department Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

The optical properties of congruent lithium niobate are analyzed from first principles. The dielectric function of the material is calculated within time-dependent density-functional theory. The effects of isolated intrinsic defects and defect pairs, including the Nb_{Li}^{4+} antisite and the Nb_{Li}^{4+}–Nb_{Nb}^{4+} pair, commonly addressed as bound polaron and bipolaron, respectively, are discussed in detail. In addition, we present further possible realizations of polaronic and bipolaronic systems. The absorption feature around 1.64 eV, ascribed to small bound polarons [1], is nicely reproduced within these models. Among the investigated defects, we find that the presence of bipolarons at bound interstitial-vacancy pairs Nb_V–V_{Li} can best explain the experimentally observed broad absorption band at 2.5 eV. Our results provide a microscopic model for the observed optical spectra and suggest that, besides Nb_{Li} antisites and Nb and Li vacancies, Nb interstitials are also formed in congruent lithium-niobate samples [2].

[1] O. F. Schirmer *et al.*, J. Phys.: Condens. Matter **21**, 123201 (2009).
[2] M. Friedrich *et al.*, Phys. Rev. Materials **1**, 054406 (2017).

KFM 27.10 Thu 15:00 Poster E

Broadband transient absorption spectroscopy of reduced lithium niobate after pulse excitation — •Stefan Hagedorn, Simon Messerschmidt, and Mirco Imlau — Department of Physics, Osnabrück University, Barbarastr. 7, 49076 Osnabrück, Germany

It is well known that transient absorption in lithium niobate (LN) can be studied by the use of single line pump and probe laser pulses [Imlau, M. *et al.*, Appl. Phys. Rev. 2 (2015)]. However, this technique inhibits access to the specific broadband absorption features of the underlying polaron species.

We have addressed this problem by installing a transient absorption spectrometer with a ns pulse laser as excitation source and a ns supercontinuum pulse laser ($\lambda = (400 - 1600)$ nm) as a probing source. Our setup is able to obtain temporal dynamics in the orders $(10^{-7} - 10^{3})$ s using an electronic delay between pump and probe pulses. For the first time we are able to show that the induced change of absorption in thermally reduced LN exhibit a transparency in the blue spectral region due to the depleted bipolarons and a significant absorption in the near-infrared induced by bound polarons. However, absorption maxima and minima are shifted from their denominated wavelengths compared to state of the art-knowledge. Using this setup, it is now possible to experimentally determine spectro-temporal absorption characteristics, e.g., to resolve polaron energy shifts caused by different pump wavelengths. This way, new insights to polaron dynamics beyond simplistic model extrapolations can be accessed. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.11 Thu 15:00 Poster E

Dynamics of small polarons in the limit of high charge carrier densities — •Thorben Groven, Simon Messerschmidt, and Mirco Imlau — Department of Physics, Osnabrück University, Barbarastr. 7, 49076 Osnabrück, Germany

Small strong-coupling polarons take a crucial part in optical processes [Imlau, M. *et al.*, Appl. Phys. Rev. 2 (2015)]; therefore, polaron dynamics in dependency of the excitation wavelength are of vital interest. Up to now, polaron excitation has been investigated in the vis-spectral range via two-photon absorption (TPA) whereas polaron dynamics initiated by higher photon energies are largely unknown.

We have addressed this question by performing systematic studies under deep UV-pulse excitation at 355 nm and probed with different cw-lasers via transient absorption spectroscopy. Optical excitation and recombination of small polarons is analyzed in terms of pump-intensity and temperature in congruent, Mg-, and Fe-doped lithium niobate (LN). At 355 nm, the bound/free polaron formation probability for congruent and Mg-doped LN increases towards the UV region because of a growing TPA coefficient, whereas iron-doped LN exhibits a decreased bound polaron formation probability altogether compared to an excitation at 532 nm due to an altered excitation path. Latter can be explained by a single photon absorption (SPA) from the valence band into the Fe^{3+}-state forming hole-polarons and Fe^{2+}. Furthermore, SPA quenches TPA and therefore, band to band transitions are suppressed. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.12 Thu 15:00 Poster E

Surface acoustic wave propagation in monoclinic ferroelectric phases in strained $K_{0.7}Na_{0.3}NbO_3$ thin films — •Jutta Schwarzkopf[1], Leonard von Helden[1], Sijia Liang[2], Roger Wördenweber[2], and Martin Schmidbauer[1] — [1]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, Berlin, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany

Formation of ferroelectric phases with monoclinic symmetry is expected to result in enhanced piezoelectric properties. Together with high coupling coefficients, this feature can be exploited for thin film surface acoustic wave (SAW) devices. $K_xNa_{1-x}NbO_3$ represents a suitable material system that does not only provide high coupling coefficients. In addition, monoclinic phases can be stabilized in thin films

by applying anisotropic epitaxial strain. Though as known from previous studies [1], the formation of the monoclinic phase crucially depends on the incorporated lattice strain. In this work, 30 nm $K_{0.7}Na_{0.3}NbO_3$ films were grown epitaxially on (110) $TbScO_3$ and (110) $GdScO_3$ substrates by metal-organic chemical vapor deposition. The films exhibit a compressive strain state with pseudocubic $(001)_{pc}$ surface orientation and periodically arranged ferroelectric stripe domains. Piezoresponse force microscopy and x-ray diffraction reveal a domain periodicity of $40 - 50$ nm and domains walls that proceed along the $[11\overline{2}]$ or $[1\overline{1}\overline{2}]$ directions of the orthorhombic substrates. These films were used for SAW experiments. Differences in SAW propagation will be discussed with regard to the symmetry of different monoclinic phases.

[1] J. Schwarzkopf et al., Front. Mater. 4, 26 (2017)

KFM 27.13 Thu 15:00 Poster E

Wavevector dependent optical properties from wavevector independent ab initio conductivity tensor — •René Wirnata[1], Ronald Starke[1], Giulio Schober[2], and Jens Kortus[1] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen

In ab initio materials physics it is common practice to consider the conductivity tensor $\sigma(\boldsymbol{k},\omega)$ in the optical limit, i.e. $\boldsymbol{k} \to \boldsymbol{0}$. However, response functions are naturally functions of both wavevector and frequency. Using *Universal Response Relations* [1], we are able to construct e. g. a frequency and wavevector dependent dielectric tensor from a wavevector independent optical conductivity. Since the dielectric function and the refractive index are related by $n^2 = \varepsilon$, we can thus calculate ab initio ordinary and extra ordinary refractive indices, $n_e(\omega)$ and $n_o(\omega)$, of birefringent materials that fit very well with experimental results from [2]. In fact, obtaining the scalar functions $n_e(\omega)$ and $n_o(\omega)$ from a dielectric tensor $\varepsilon(\boldsymbol{k},\omega)$ requires in the most general case a more sophisticated algorithm, which is already known in theoretical optics [3-4]. In order to illustrate the reliability of this approach for different materials types, we have chosen Si, TiO_2 and α-Quartz as examples for isotropic, birefringent and optically active crystals.

[1] R. Starke, G.A.H. Schober: Photonic.Nanostruc. **14** (2015)
[2] E. Palik: Handbook of Optical Constants of Solids (2002)
[3] H. Römer: Theoretische Optik, Wiley-VCH (1994)
[4] R. Starke, G.A.H. Schober: arXiv:1708.06330

KFM 27.14 Thu 15:00 Poster E

Construction of a broadband Sub-THz-Spectrometer — •Max Pargmann, Christoph Grams, and Joachim Hemberger — Universität zu Köln

Between the highest frequencies that are accessible with conventional dielectric spectroscopy (≈2E10 Hz) and the lowest in optical free-beam spectroscopy (≈2E11 Hz), measurements are difficult due to technical limitations [1]. We try to close this frequency gap by building a new time-domain spectrometer enabling us to measure a wide frequency range starting from 5 GHz up to 500 GHz. We use a pulsed laser setup with a variable delay up to 500 ps combined with a pulse picker to customize the average optical power. For measurement, we use an on-chip emitter detector design in microstrip geometry, with embedded GaAs photoconductive switches, which allows for generation and detection of pulses ≈ 300 fs [2]. The spectrometer is compact and complete fiber based therfore it can be easily implimentated in commerical magneto cryostats without the need of free beam.

This work is supported by the Deutsche Forschungsgemeinschaft via SFB1238 (Cologne).

[1] C. Matheisen et al, IEEE Xplore 15598877(2015)
[2] M.B. Byrne et al, Appl. Phys. L93, 182904 (2008)

KFM 27.15 Thu 15:00 Poster E

Optimising interferometric displacement detection for NC-AFM operation — •Alexander von Schmidsfeld and Michael Reichling — Universität Osnabrück

We systematically describe the steps needed for optimal calibration of interferometric displacement detection of the cantilever in NC-AFM and demonstrate that the interferometer for displacement detection can be operated in both, the Michelson and the Fabry-Perot mode. After describing the basic interferometer setup, we present a method to characterize the optical losses occurring in the feed line and the results of deficient fiber-cantilever alignment. Furthermore, we introduce the method of 3D intensity mapping of the optical cavity response and recordings of the interferometer signal as a function of the fiber-end-to-cantilever distance, both together allowing us to optimize the adjustment. Finally we examine the impact of opto-mechanical effects occurring in a cavity of sufficient finesse on the detection noise figures and the effective parameters of the cantilever oscillation, namely the Q-factor Q0 and the stiffness k0, both split into values for positive and negative fringes of the interferogram, respectively.

KFM 27.16 Thu 15:00 Poster E

Limitations of Single-Step Phase Retrieval — •Johannes Hagemann[1,2], Mareike Töpperwien[1], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]current address: DESY, X-Ray Nanoscience and X-Ray, Optics, Notkestraße 85, 22607 Hamburg

In order to harness the full information of propagation-based phase contrast images obtained with coherent x-rays, one has to carry out a phase reconstruction on the images. This strategy is applied for data obtained in various optical regimes ranging from the edge enhancement to the deeply holographic regime.

By placing assumptions on the specimen e.g. weak absorption one can construct several single-step solutions for the respective optical regime. Despite the merrits of these schemes, the reconstruction obtained is only as good as the assumptions hold.

We demonstrate on an example near-field hololographic dataset, the flaws of the single-step reconstruction based on the contrast transfer function[1] and the possible improvement gained by applying an iterative reconstruction scheme.

[1] P. Cloetens et al., Appl. Phys. Lett.(1999), **75**, 2912*2914.

KFM 27.17 Thu 15:00 Poster E

In situ gas-cell for the analysis of sorption behavior on surfaces by using X-ay fluorescence and absorption spectrometry under total reflection geometry — •Cornelia Streeck[1], Daniel Grötzsch[2], Jan Weser[1], Wolfgang Malzer[2], Andreas Nutsch[3], Thomas Wiesner[1], Birgit Kanngiesser[2], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — [2]Technische Universität Berlin and Berlin Laboratory of innovative X-ray Technologies, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Helmut Fischer GmbH, Industriestraße 21, 71069 Sindelfingen

A novel measuring cell for in-situ metrology of molecules of light elements e.g. volatile organic compounds and their sorption behavior on different surfaces was developed. The cell is designed for the soft X-ray range (especially C, N, and O) and is constructed for flow-through operation in a high-vacuum chamber. It allows for the analysis of the surface under total reflection geometry with Total-Reflection X-Ray Fluorescence (TXRF) analysis and X-ray Absorption Spectroscopy (XAS). First experiments using ethanol on steel and Si-wafer surfaces were applied.

KFM 27.18 Thu 15:00 Poster E

Detection of electronic anisotropies in cuprates by precision x-ray polarimetry with quartz crystals — •Annika Tamara Schmitt[1,2], Ingo Uschmann[1,2], Kai Sven Schulze[1,2], Robert Lötzsch[1,2], Hendrik Bernhardt[1,2], Benjamin Grabiger[1,2], Berit Marx-Glowna[2,3], Yves Joly[4], Martin von Zimmermann[3], Hasan Yavas[3], Hans-Christian Wille[3], Eckhart Förster[2], Gerhard Paulus[1,2], and Ralf Röhlsberger[3] — [1]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany — [2]Helmholtz-Institut Jena, Helmholtzweg 4, D-07743 Jena, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg, Germany — [4]Institut Néel , 25 Avenue des Martyrs, F-38042 Grenoble, France

To understand the origin of the high-temperature superconductivity in the cuprates, it is necessary to study the electronic structure of the copper oxides. Information about the electronic structure and symmetry can be obtained by XANES measurements at the Cu K-edge. The combination of x-ray spectroscopy and x-ray polarimetry offers a much more sensitive method to explore electronic anisotropies and magnetic moments, since the absorption depends on the polarization state.Using crossed x-ray polarizers, tiny optical anisotropies caused by electronic anisotropies can be detected. The x-ray polarizers are based on Bragg reflection at scattering angles very close to 90°. Polarization purities up to $1.2 \cdot 10^{-7}$ can be reached using quartz polarizers with a 320-reflection at the Cu K-edge.

KFM 27.19 Thu 15:00 Poster E

XAFS by an X-ray tube based laboratory spectrometer — •Sebastian Praetz[1], Christopher Schlesiger[1], Lars

Anklamm[1,3], Holger Stiel[2], Wolfgang Malzer[1], and Birgit Kanngiesser[1] — [1]Institute for Optics and Atomic Physics, Technical University Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Max-Born-Insitut, Max Born-Straße 2a, 12489 Berlin, Germany — [3]IAP e.V., Rudower Chaussee 29/31, 12489 Berlin, Germany

The spectroscopy of X-ray Absorption Fine Structure (XAFS) is a frequently used method for the investigation of the electronic structure or for the identification of chemical compounds, such as the oxidation state or coordination of functionalized materials. This technique is usually performed at synchrotron radiation facilities because of the need of a brilliant X-ray source and a high spectral resolving power. A laboratory setup would have the advantage of higher accessibility and flexibility, which would open this technique for routine analysis.

In this contribution, we will present our successfully developed X-ray tube based von Hamos laboratory XAFS spectrometer using a novel type HAPG mosaic crystal with a spectral resolving power up to $E/\Delta E = 4000$ and a wide energy range of 4 keV to 12 keV.

We are able to measure liquid as well as solid state samples in transmission. Usual acquisition times are in the range of a few minutes to several tens of minutes. First applications will be shown, e.g. the identification of oxidation states. These results are very promising and show the capability of this spectrometer for all kinds of XAFS measurements.

KFM 27.20 Thu 15:00 Poster E

3D reconstruction from one-dimensionally blurred projections — •Leon Merten Lohse, Malte Vassholz, and Tim Salditt — Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Although high-brilliance radiation sources become more and more available, many applications are depending on laboratory x-ray sources or neutron sources with low brilliance. Due to the low brilliance, a trade-off between high resolution and feasible acquisition time has to be made. The use of 1D (line) sources has been demonstrated recently, to be able to increase the flux without any impact on the resolution and thus circumvent the trade-off [1,2]. A particularly simple method, which is based on the 3D Radon transform, can be used to reconstruct the 3D volume from a set of projections from a line source. If the divergence of the beam can be neglected, the planar integrals required for the 3D Radon transform can be directly extracted from the projections, and a 3D analogon to the well-known filtered-back-projection algorithm can be formulated.

[1] L. M. Lohse et al. "Tomography with extended sources: ...", Phys. Rev. A (accepted 11/2017) [2] M. Vassholz et al. "New X-Ray Tomography Method ... ", Phys. Rev. Lett. (2016)

KFM 27.21 Thu 15:00 Poster E

X-ray emission spectroscopy (XES) by an X-ray tube based laboratory spectrometer — •Richard Gnewkow[1], Christopher Schlesiger[1], Daniel Grötzsch[1], Lars Anklamm[2], Fabian Kowalewski[3], Serena DeBeer[3], Wolfgang Malzer[1], and Birgit Kabbgiesser[1] — [1]Institute for Optic and Atomic Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für angewandte Photonik e. V. (IAP), Rudower Chaussee 29/3, 12489 Berlin, Germany — [3]Max Planck Institute for Chemical Energy Conversion, Stiftstr. 34 - 36, 45470 Mülheim a.d. Ruhr, Germany

X-ray emission spectroscopy (XES) is an upcoming method for the investigation of the electronic structure of chemical compounds. Typically the chemical shift of the Kβ-multiplett is analyzed. XES, therefore, requires a high spectral resolution and is mainly performed at synchrotron facilities.

We developed an X-ray tube based laboratory spectrometer for XES experiments. The dispersive element is a graphite mosaic crystal called Highly Annealed Pyrolytic Graphite (HAPG) in an adapted von Hamos geometry. The full cylinder optic combines high efficiency with a spectral resolving power of $E/\Delta E = 4000$ for an energy range between 2 keV - 10 keV. The use of a polycapillary lens allows the analysis on a micrometer scale.

In this contribution, we will present the setup of the spectrometer and its properties. We will show results for the Kβ diagram line and valence-to-core region for thin and diluted samples, e.g. catalysts.

KFM 27.22 Thu 15:00 Poster E

X-ray fluorescence and X-ray diffraction analysis of a historical painting — •Fatima Mallal[1], Alex von Bohlen[2], Christian Sternemann[1], Michael Paulus[1], Anne Hüsecken[1], Paul Salmen[1], Wolf-Dieter Köster[3], Jörg Hansen[4], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Germany — [2]Leibniz-Institut für Analytische Wissenschaften ISAS, Germany — [3]Dortmund, Germany — [4]Bachhaus Eisenach, Germany

According to the current state of knowledge, there are only two paintings of Johann Sebastian Bach (1685-1750) which were made during his life time. Both are exhibited in the *Bach House* in Eisenach. We present an X-ray fluorescence (XRF) and X-ray diffraction (XRD) study on a third painting of unspecified origin in order to proof its authenticity, which was performed at beamline BL 9 of DELTA synchrotron radiation source. The XRF data was used to detect the elemental composition of the painting, whereas the XRD pattern provide insight into the crystal structure of colors and pigments. This analysis enables to draw conclusions about the age of the painting, as specific colors are characteristic for certain ages.The XRF analysis showed a predominant contribution of the elements lead, zinc, calcium and barium. We identified the pigments lead white (2PbCO3 Pb(OH)2), lithopone (BaSO4 ZnS), and low amount of zinc white (ZnO) at different regions of the painting. Moreover chalk (CaCO3) was detected. The observation of the different pigments indicates that corrections of the portrait have been made in the 19th century.

KFM 27.23 Thu 15:00 Poster E

Harmonic nanoparticles as markers for in-vivo imaging — •Dustin Dzikonski[1], Christian Kijatkin[1], Kay Lammers[2], Achim Paululat[2], and Mirco Imlau[1] — [1]Department of Physics, Osnabrück University, Germany — [2]Department of Zoology & Developmental Biology, Osnabrück University, Germany

Nanoscaled optical markers are versatile contrast agents in biological environments; especially fluorescing dyes have risen to a microscopy standard. However, rather rigid excitation-emission wavelengths as well as Stokes shifts towards the red spectrum pose severe limitations to this class of materials. Moreover, time-critical analysis is hindered due to photobleaching, blinking, and potentially long fluorescent lifetimes.

A solution is the use of harmonic, alkali niobate-based nanoparticles that offer unprecedented flexibility due to their photostability, instantaneous response, and frequency tunability in a vast range [C. Kijatkin *et al.*, *Photonics* **2017**, *4*(1), 11]. In light of novel applications, we plan to utilize infrared radiation from femtosecond pulsed lasers in combination with harmonic generation to i) increase excitation depth due to the lower absorption in this range, ii) create visible up to UV light for detection and manipulation, and iii) allow for time-critical evaluation of dynamic systems. As a proof of principle, we present our studies on using lithium niobate nanoparticles as tracers via second harmonic generation of infrared radiation to visualize and quantify the hemolymph velocity flux inside the heart chamber of living *Drosophila melanogaster* as a model system. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.24 Thu 15:00 Poster E

Ptychography goes magnetic: Developing direct magnetic imaging with hard X-rays at PETRA III's P09 — •Florian Heinsch[1,2], Felix Wittwer[3], Sonia Francoual[3], Dennis Brückner[3], Maik Kahnt[3], Martin Seyrich[3], David Reuther[3], Martin Zwiebler[2], and Jochen Geck[2] — [1]HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]DESY, Hamburg, Germany

X-rays are an ideal probe for non-destructive imaging of a bulk-sample's structure, featuring high spatial resolution and possible element sensitivity. Our goal is to combine these properties with the magnetic sensitivity provided by the X-ray absorption process in order to image magnetic properties with nanometer resolution.

We present the results of a first experiment at the magnetic scattering beamline P09 of PETRA III. All additionally required components, including focusing lenses, could be successfully integrated in the beam path with a stability that allowed for conventional ptychography with a resolution of at least 60nm. Subsequently it will be possible to directly map out the XMCD of a given thin sample. Therefore the difference of two ptychograms with opposing circularly polarized light needs to be compared. First results are presented and an outlook is given on the way to imaging of magnetic domains by magnetic ptychography at PETRA III.

KFM 27.25 Thu 15:00 Poster E

Analysis of Multilayer Zone Plates (MZP) for Imaging with

hard X-Rays and Nanometer Resolution — •Jakob Soltau, Lars Melchior, Tim Salditt, and Markus Osterhoff — Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany

The brilliance of modern synchrotrons cleared the path towards generating highly focussed x-ray beams. While focal spot diameters of a few nanometers are already common at lower x-ray energies (< 10 keV), there is a lack of x-ray optics suited for scanning microscopy with small spot sizes at higher energies. The challenge for manufacturing zone plates in the hard x-ray energy range is the high aspect ratio, defined by the large optical thickness (>5 μm) - needed due to the low interaction between photons and matter - and small zone widths (<10 nm) [1]. The propagation of electromagnetic waves in structures not much larger than their wavelength and with high-aspect ratios lead to effects as waveguiding and dynamical diffraction. To assess these effects and characterize the efficiency of multilayer zone plates (MZP) 3D finite-differences simulations [2] have been performed. The simulation of the electromagnetic fields inside and behind the MZP showed the advantage of circular MZPs to achieve very high photon flux densities in a single focal point of 5 nm diameter. Furthermore the simulations were revealing interaction processes like e.g. dynamical diffraction inside the MZPs. [1] C. Eberl et al. Fabrication of laser deposited... In: Applied surface science 307 (2014) [2] L. Melchior et al. Finite difference methods for... In: Opt. Express (accepted)

KFM 27.26 Thu 15:00 Poster E

DLTPulseGenerator: A C/C++ Library for the Simulation of Lifetime-Spectra based on Detector-Output Pulses — •Danny Petschke and Torsten Staab — University Würzburg, Dep. of Chemistry, LCTM, Röntgenring 11, D-97070 Würzburg, Germany

The quantitative analysis of lifetime spectra relevant in both life- and material sciences presents one of the ill-posed inverse problems and, hence, leads to most sophisticated requirements on the hardware-specifications and -parameters of the setup as well as on the analysis algorithms. Here we present DLTPulseGenerator, a library written in native C++ 11 which provides a simulation of lifetime spectra according to the measurement setup: i.e. the kind of detectors and the acquisition hardware. The simulation is based on pairs of non-TTL detector-pulses. Those pulses require the Constant-Fraction Principle (CFD) for the determination of the exact timing signal and, thus, the calculation of the time difference i.e. the lifetime. The library provides the simulation of discrete specific lifetimes (e.g. metals, polymers) and the simulation of specific lifetime distributions (Gaussian, Lorentzian and Log-Normal) as can be found in porous materials, i.e. Vycor-glasses and aerogels. To verify our method, simulation results were visually and quantitatively compared to experimentally obtained data using Positron-Annihilation Lifetime Spectroscopy (PALS) on pure Aluminium (4N).

KFM 27.27 Thu 15:00 Poster E

Quantum electronic scattering in a Au/Co/Au nanowire lead — Adel Belayadi[1] and •Boualem Bourahla[2] — [1]University of M. Bougara, Department of Coating Material and Environmental, Boumerdes, Algeria — [2]Laboratory of Physics and Quantum Chemistry, M. Mammeri University, Tizi-Ouzou, Algeria

In the present contribution, we provide a theoretical model to investigate the electron scattering states in a one-dimensional atomic chain which contains a single defect atom. In fact, in ideal leads the translation symmetry is treated by periodic boundary conditions. However, in the case of a defect, the Bloch theorem is not applicable. In other words, the single defect atom breaks the symmetry and makes the solution of eigenvalues problem impossible. To deal with inhomogeneous systems, due to lack of symmetry, we have integrated the phase field matching theory (PFMT) to compute the eigenvalue problem of our system. The PFMT connects the left and right leads, separated by the defect atom, in terms of the total transmission and reflection probabilities of the Landauer-Büttiker formalism. As application, we build up the Hamiltonian matrix in the tight-binding approach and then we compute the coherent scattering and transport of electron as well as the electronic conductance across the defect junction given as copper/cobalt/copper, while the cobalt atom is treated as a defect atom.

KFM 27.28 Thu 15:00 Poster E

High-resolution structural and chemical analysis of transition metal oxide nanoparticles — •Aladin Ullrich, Daniel Schmidtner, Mohammad Mostafizar Rahman, and Siegfried Horn — University of Augsburg, 86159 Augsburg, Germany

We have investigated the structural and chemical composition of pure iron oxide and manganese ferrite nanoparticles by transmission electron microscopy (TEM). The particles were synthesized by thermal decomposition of the corresponding metal oleate salts in high-boiling solvents. Na-oleate was used as surfactant for shape control during the synthesis.

The synthesized particles are 20nm in size and appear core-shell like in bright field TEM images. High-resolution TEM (HRTEM) analysis reveals a FeO/MnO like structure in the core and a spinel like structure in the shell.

To resolve the spatial distribution and the oxidation state of the metals manganese and iron within the particles, high-resolution energy loss spectroscopy (EELS) and energy dispersive x-ray spectroscopy (EDS) were performed.

Iron and manganese show differences between their oxidation state in the core and the shell region of the particles. This is consistent with the structures observed in HRTEM analysis. The oxidation state of the iron ions is lower in the core than in the shell region. For manganese ions, only a thin surface layer shows different oxidation state. Traces of sodium used as surfactant during the synthesis were detected on the surface of the particles.

KFM 27.29 Thu 15:00 Poster E

Electro-osmotic pumping for structured coatings — •raheema muhammad aslam, Ran Niu, and Thomas Palberg — Institute of Physics, JGU Mainz, Germany

We assemble charged colloidal spheres at deliberately chosen locations on a charged unstructured glass substrate utilizing ion exchange based micro-pumps. The pump uses trace amounts of ions to generate electro-osmotic fluid flows. We show experimentally that our pump operates in almost deionized water for periods exceeding 24 h and induces fluid flows in micrometer per second over hundreds of micrometers. This flow displays a far-field, power-law decay which is characteristic of two-dimensional (2D) flow when the system is strongly confined and of three-dimensional (3D) flow when it is not. Experimentally, we systematically explore the control parameters of crystal assembly at and by micro-pumps and the mechanisms through which they depend on the experimental boundary conditions. We demonstrate that crystal quality depends crucially on the assembly distance of the colloids. This is understood as resulting from the competition between inward transport by the electro-osmotic pump flow and the electro-phoretic outward motion of the colloids. Optimized conditions include substrates of low and colloids of large electro-kinetic mobility. Then a sorting of colloids by size is observed in binary mixtures with larger particles assembling closer to the ion exchanger beads. Moreover, mono-sized colloids form defect free single domain crystals which grow outside a colloid-free void with facetted inner crystal boundaries centred on the ion exchange particle.

KFM 27.30 Thu 15:00 Poster E

Cladding-like waveguide structure in Nd:YAG crystal fabricated by multiple ion irradiation for enhanced waveguide lasing — •zhen shang[1,2], shengqiang zhou[1], and yang tan[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]School of Physics Shandong University, Jinan, China

we report on a cladding-like waveguide structure in Nd:YAG crystal fabricated by the multiple carbon ion beam irradiation. After the designed multiple irradiation process, the cladding-like waveguide with triple refractive-index layers were constructed in the region near the surface of the crystal. With such a structure, the waveguiding core was compressed and refractive index profile was modified, resulting in a higher light intensity than that of the single ion-beam-irradiated monolayer waveguide. The waveguide lasing at wavelength of 1064 nm was achieved with enhanced performance in the cladding-like structures with both planar and ridge configurations by the optical pump at 810 nm.

KFM 27.31 Thu 15:00 Poster E

Crystallisation of Bismuth in an Inert Atmosphere and Electrical Characterization of these Crystals — •Christian Düputell, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

The aim of this work is to validate diverse melting processes for the

growing of bismuth crystals in different gas atmospheres (purity of used Bi: 99,99%). Therefore, melting in two different atmospheres has been performed; in air and in an inert atmosphere (argon). The methods were assessed in terms of characterisation of the grown crystals; for this purpose, the crystals were examined visually as well as electrically.
A particular advantage of an inert atmosphere is the prevention of oxidation of the growing crystals. This leads to the formation of purer, larger as well as more distinct bismuth crystals. The observation has been proven in two different ways: first by a visual characterisation of the crystals using a light microscope and second by Hall-Effect measurements of selected crystal samples. The results of the Hall-Effect measurements demonstrate the particular electrical and magnetic properties of the half-metal bismuth. At room temperature, the measured Hall-coefficient of crystals formed in the air is about $-9,64(30) \cdot 10^{-9}$ m^3 C^{-1} in comparison to $-9,42(16) \cdot 10^{-7}$ m^3 C^{-1} of crystals formed in an inert atmosphere.
Furthermore, a modification of the so called "Czochralski process" has been examined. So in future works it may be possible to improve the forming of bismuth single crystals without manual intervention.

KFM 27.32 Thu 15:00 Poster E

The Influence of Rare Earth Doping and Co-doping of ZnO Nanoparticles on Structural and Optical Properties — •Maria Toma[1,2], Oleksandr Selyshchev[3], Aurel V. Pop[1], and Dietrich R.T. Zahn[3] — [1]Babes-Bolyai University, Physics Faculty, M. Kogalniceanu No. 1, 400084, Cluj-Napoca, Romania — [2]Research Center for Advanced Medicine Iuliu Hatieganu University of Medicine and Pharmacy, Cluj-Napoca, Romania — [3]Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Gd-doped, Er-doped, and (Gd+Er) co-doped ZnO nanocrystals were prepared by a soft colloidal synthesis method [1]. Due to their applications in optoelectronic, display, and memory devices [2,3], semiconductor nanocrystals doped with rare earths (RE) are of great interest. Microstructural properties of the nanocrystals obtained were characterized using Raman spectroscopy and their distribution and crystallinity were identified using transmission electron microscopy. From TEM measurements we evaluated the size of the nanoparticles to be in the range of 4 to 7 nm. Optical properties were investigated using photoluminescence (PL) and UV-vis spectroscopy to understand the excited state energy distribution between band to band transitions and the defect states. Depending on the size distribution of the nanoparticles, changes in the PL and UV absorbance of ZnO were observed, due to the incorporation of RE ions into the ZnO nanostructure Owing to the electronic configuration of the RE ions, the 4f shell transitions show sharp and narrow band emission. This effect is consistent with Raman and other literature results.

KFM 27.33 Thu 15:00 Poster E

Discovery of a high-pressure RuCl3 phase with complete cation disorder — •Lisa Leissner, Ulrich Bläss, Marcus Schwarz, and Edwin Kroke — Tu Bergakademie Freiberg, Freiberg, Germany

The alpha form of Ruthenium(III)-chloride is a hot topic in spin liquid physics because it is one of the most promising materials to realize the Kitaev model of a quantum spin liquid. It fulfills the criteria for realizing the Kitaev interactions (Jackeli & Khaliullin 2009, Glamazda et al 2017). At low temperatures, it orders to a zigzag magnetic order. However, in Raman spectroscopy as well as inelastic neutron scattering some hints of spin liquid physics could be observed (Sears et al, 2017). The transition temperature is strongly dependent of the sample, especially its stacking faults. The effective magnetic interactions between the Ru-moments strongly depend on the distance and Ru-Cl-Ru angle. Hence, a change of one of these parameters, as e.g. occurring after second order phase transitions, may change the ratio between Kitaev and Heisenberg interactions. In order to explore such potential transitions, we have conducted various heated and unheated high pressure experiments to explore stable or metastable high-pressure phases of RuCl3. Multianvil experiments led to the formation of single crystals of a new RuCl3 phase. Single crystal X-ray diffraction revealed a small unit cell with space for two atom sites only, while spectroscopic measurements indicate that a Ru:Cl ratio of 1:3 is still present. We thus have synthesized a new and possibly metastable hexagonal form of RuCl3 with a completely random occupation of one third of the cation site.

KFM 27.34 Thu 15:00 Poster E

Single-crystal diffractometers HEiDi and POLI at MLZ: (Un)polarised neutrons to probe crystallographic and magnetic domains — •Andrew Sazonov[1,2], Martin Meven[1,2], Vladimir Hutanu[1,2], and Georg Roth[1] — [1]RWTH Aachen, Institute of Crystallography, D-52056 Aachen, Germany — [2]Jülich Centre for Neutron Science at MLZ, D-85748 Garching, Germany

HEiDi and POLI are the only single-crystal neutron diffractometers in Germany and two of the very few in the world which are located at a hot neutron source to enlarge the flux of neutrons with short wavelengths. It allows to minimize the absorption problems associated with certain elements and to explore extremely large portions of reciprocal space. HEiDi is a typical 4-circle diffractometer with Eulerian cradle for detailed studies on crystal and magnetic structures in the temperature range 2.5–1300 K. POLI is an independent diffractometer, which extends the possibilities of HEiDi to the milli-Kelvin range and external magnetic fields as well as offers in addition different types of polarized neutron techniques: Flipping-ratio measurements in applied magnetic field for ferromagnetic and paramagnetic materials and spherical neutron polarimetry in zero field for more complex magnetic structures. Due to their possibilities, both instruments contribute to many topics, e.g. in the energy and information sector. Here, on examples of multiferroic and superconducting materials, we give an overview of the instruments possibilities in studying of crystal and magnetic structures and phase transitions of solids in general, and their crystallographic and magnetic domains (microstructures) in particular.

KFM 27.35 Thu 15:00 Poster E

The crystal structure of trisodium hexachloroiridate — •Martin Etter[1], Melanie Müller[2], and Sebastian Bette[3] — [1]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]Universität Duisburg-Essen, Duisburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Strongly hygroscopic inorganic compounds exhibit a rich field of unsolved crystal structures as often several hydrated forms exist. However, solving these crystal structures is challenging, since single crystals are in many cases not available and powders usually consist of several hydrated phases at the same temperature and moisture conditions. Such a challenging compound is for instance the highly hygroscopic trisodium hexachloroiridate (Na3IrCl6) which possess multiple hydrated phases and a so far unsolved crystal structure even of the anhydrous phase.

Here, the crystal structure of the anhydrous phase of trisodium hexachloroiridate (Na3IrCl6) at room temperature was solved after a dehydration process using laboratory powder X-ray diffraction. It was found that the crystal structure of Na3IrCl6 crystallizes in space group P-31c isostructural to the crystal structures of Na3CrCl6, Na3InCl6 and Na3MoCl6 as well as to recently found crystal structure of trisodium hexachlororhodate (Na3RhCl6).

In this presentation structural details about the dehydrated compound will be given as well as an outlook to the variety of hydrated phases.