KFM 14: Postersession KFM

Time: Wednesday 16:00–18:30 Location: Poster C

KFM 14.1 Wed 16:00 Poster C

Fabrication of polymeric Whispering-Gallery-Mode resonators on tunable liquid crystal elastomer substrates using Deep-UV — •Lukas Mall, Simon Woska, Jannis Hessenauer, Carolin Klusmann, Tobias Siegle, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) micro resonators offer huge potential for future applications in photonic devices. For many applications, a cheap and upscalable production is indispensable, which requires the development of reproducible and fast production processes. Polymers as resonator material open up the possibility to structure WGM resonators using Deep-UV lithography. This method allows parallel production of a large number of resonators at low costs.

Polymers also allow implementation of flexible photonic components like photonic molecules with a tunable inter-cavity gap. Such elements are achieved by structuring WGM resonators on flexible substrates. Especially promising substrates are made from liquid crystal elastomers (LCEs) which show thermally induced geometrical modifications.

In this contribution, we detail the production process of DUV-structured high-Q WGM resonators made from poly (methyl methacrylate) (PMMA) on LCE substrates. To overcome problems regarding stability, adhesion, process reliability etc., we employ stacked layers of several different polymers utilizing their very own characteristics.

KFM 14.2 Wed 16:00 Poster C

Tunable Whispering-Gallery-Mode Resonators made from Liquid Crystal Elastomers — •Jannis Hessenauer, Carolin Klusmann, Simon Woska, Matthias Migeot, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Whispering-Gallery-Mode resonators are promising building blocks for the realization of photonic devices, such as optical filters, switches or modulators. For a proper performance of these devices, a high tunability of their components is required. To achieve this, we propose resonators made from Liquid Crystal Elastomers (LCEs) as a novel way to tune their resonance wavelength over a wide spectral range.

Their working principle is based on a thermally induced reversible phase transition of LCEs from a nematic to an isotropic phase, which changes the resonator dimension, and therefore the resonance wavelength. LCEs are aligned through a silanization process and LCE resonators are structured using Direct Laser Writing (DLW). To induce the phase transition and the resulting shape deformation, the LCE resonators are doped with an absorber dye. The latter allows heating individual resonators via laser illumination.

To demonstrate reversible tuning of the resonance wavelength, the temperature dependent mode spectra of LCE resonators are evaluated. Heating of the resonators leads to a partly reversible redshift of more than one Free Spectral Range (FSR). The underlying increase in resonator radius can also be used to enable tunable coupling of adjacent resonators in photonic molecules.

KFM 14.3 Wed 16:00 Poster C

Wide Tunability of Coupled WGM Resonators Using Flexible Elastomer Substrates — •Simon Woska, Lukas Mall, Jannis Hessenauer, Carolin Klusmann, Tobias Siegle, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Whispering-Gallery-Mode (WGM) resonators are promising building blocks in photonic devices like optical filters or Coupled Resonator Optical Waveguides (CROWs). Contrary to common implementations of WGM resonators using silica as resonator material, we focus on polymers, which allow for a low-cost and upscalable production.

For plenty of photonic applications a tunable inter-cavity gap between different resonators is highly demanded. These properties can be achieved using flexible substrates, such as elastomers.

Flexible tuning of the inter-cavity gap has been successfully realized in our research group using a mechanically deformable elastomer as substrate. In this contribution, we propose a system based on substrates made from Liquid Crystal Elastomers (LCEs). Due to a phase transition at rather low temperatures, LCE undergoes a fully reversible change in dimension when heated. Thanks to this feature, LCE substrates exhibit several advantages compared to mechanically deformable substrates, including a more adjustable actuation.

We demonstrate the advantages of LCEs over the established mechanically deformable substrates and propose different approaches for the realization of such a tunable system. First results of coupled high-Q WGM resonators structured on LCE substrates are presented.

KFM 14.4 Wed 16:00 Poster C

Non-Hermitian Defect States from Lifetime Differences — •Marti Bosch — TU Ilmenau, Ilmenau, Germany

The existence of non-hermitian defect states in optical systems is known for systems of coupled resonators with asymmetric backscattering. Here, we demonstrate that defect states in open optical systems can exist due to lifetime differences of counterpropagating modes without the need for asymmetric backscattering within the single resonator. We apply our findings to a finite system of coupled resonators perturbed by nanoparticles, in which we create an interface by inverting the orientation of the resonators in half of the chain. We compare a tight-binding approximation to a full-wave numerical simulation, showing that a system with spectrally isolated defect states can be implemented in a non-hermitian photonic device.

KFM 14.5 Wed 16:00 Poster C

Dielectric properties of P(VDF-HFP)/Ceramic Composites with Respect to Energy Storage Applications — •Marius Falkenstein[1], Tino Band[1], Till Mälzer[1,2], Hartmut S. Leipner[1], Stefan G. Ebbinghaus[1], Kathrin Dörr[1], and Martin Diestelhorst[1] — [1]Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06099 Halle, Germany — [2]enspring GmbH, Weinbergweg 23, 06120 Halle, Germany

Efficient energy storage is necessary for continuous power supply and mobile applications based on alternative energy sources. Because of their high power densities capacitors are interesting for this purpose. Ferroelectric P(VDF-HFP) is a promising storage material, since it exhibits a permittitvity much higher than commonly used polymers.

Within this work, we investigated the pure P(VDF-HFP) as well as nanocomposites of this polymer with powders of TiO_2 and $BaTiO_3$, two ceramics with high permittivities. The dielectric properties of these materials were analyzed with respect to the concrete demands for energy storage.

Besides the frequency dependence of the permittivity and loss at low fields we studied the behavior at high electric fields. Cyclic unipolar D-E-measurements at low frequencies were used to separate conductivity from dielectric properties and to determine the energy-density stored at the capacitors as well as breakdown fields. All these properties were characterized concerning their dependence on the concentration of the fillers and on temperature.

KFM 14.6 Wed 16:00 Poster C

A low cost potassium Prussian blue cathode for potassium ion batteries — •Chenglin Zhang, Yang Xu, Long Liu, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Potassium-ion batteries (PIBs) have attracted increasing attention as a promising alternative to lithium-ion batteries. The hydrated potassium Prussian blue, K0.220Fe[Fe(CN)6]0.805, as a potential cathode material is first demonstrated in PIBs. The cathode exhibits a large reversible capacity within a high and flat potassiation potential of 3.1~3.4 V as well as a great cyclability. Electrochemical reaction mechanism analysis identifies the carbon-coordinated FeIII/FeII couple as redox-active site and proves structural stability of the cathode during charging/discharging. Furthermore, we present a PIB full-cell by coupling the Prussian blue nanoparticles with commercial carbon materials, which confirms the value of practical applications.[1] Considering the low cost and material sustainability, this work is of great significance for the future research and commercial applications of PIBs electrode materials.

[1] Chenglin Zhang, Yang Xu, Min Zhou, Liying Liang, Huishuang Dong, Minghong Wu, Yi Yang, and Yong Lei*[J] Adv. Funct. Mater. (2017):1604307.

KFM 14.7 Wed 16:00 Poster C

Polarization dependent vibrational properties of the ferroelectric $LiNbO_3$(0001) surfaces — •Mike Nico Piontеck, Christof Dues, Kris Holtgrewe, and Simone Sanna — Justus-Liebig-Universität Gießen

The investigation of the vibrational properties has recently become one of the most appealing tools for surface analysis. As Raman frequencies as well as selection rules are strongly related to the surface structure, they represent reliable criteria to identify, validate or rule out competing structural models [1].

In this work, we model the vibrational properties of ferroelectric $LiNbO_3$ surfaces from first principles. The $LiNbO_3$(0001) surfaces are both of technological and academic interest [2], however, the determination of the polarization direction is usually performed by destructive (chemical etching) or elaborate methods that exploit the pyroelectric or piezoelectric properties of the material. Our calculations reveal the presence of surface localized and polarization specific phonon modes of different symmetry in the frequency range between 30 and 960 cm^{-1} both at the positive and at the negative $LiNbO_3$(0001) surface. Calculated Raman intensities demonstrate that most of the surface localized modes are Raman active.

Raman spectroscopy can be thus considered as an easier to implement and non-destructive method to determine the polarity of $LiNbO_3$ surfaces.

[1] B. Halbig et al., Phys. Rev. B 97, 035412 (2018) [2] S. Sanna et al., J. Phys.: Condens. Matter 29, 413001 (2017)

KFM 14.8 Wed 16:00 Poster C

PSF-analysis of ferroelectric domain-walls in tightly focused regimes — •Peter Mackwitz, Kai Spychala, Alex Widhalm, Christof Eigner, Christine Silberhorn, Gerhard Berth, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

A combined experimental and numerical approach is applied to unravel the second-harmonic generation contrast mechanism of ferroelectric domain structures. The numerical calculation comprises a vectorial model of the imaging process. Experimentally we use a direct imaging technique which records the spatial distribution of the second-harmonic signal in the back focal plane. As the model depends on the optical properties of the material different scenarios of contrast mechanisms can be simulated and compared to the experimental data. With lithium niobate and potassium titanyl phosphate as model systems it turns out that many features of the nonlinear signatures of ferroelectric domain boundaries arise from destructive interference of phase-shifted wavelets. The phase is acquired due to the interaction of the focus with differentially poled domains, whose susceptibility tensor appears rotated by 180°. Another ingredient for the contrast are new tensor elements which do only occur at the domain walls. Furthermore, incoherence due to wall roughness plays an important role. Considering those three phenomena the contrast mechanism can be well described and predictions for other material systems become possible.

KFM 14.9 Wed 16:00 Poster C

Loss tangent mapping measurement on large area diamond discs - An approved quality control method — •Andreas Meier and Theo Scherer — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

As part of electron cyclotron development for heating of several fusion experiments (W7X, Asdex Upgrade, ITER) the characterization on bare and brazed polycrystalline chemical vapour deposition (CVD) diamond discs has been performed. An overview of dielectric properties particularly the loss tangent on about 70 different large area torus and gyrotron windows (Ø80mm - 140mm) realised with low power open resonators is shown. A spherical resonator is used for high-resolution measurements (loss tangent 10E-6) at the centre of the disc. Quality control measuring relating to the homogeneity has been realised with a hemispherical mapping setup (spherical and plane mirror). The results are given in statistic value D10 (10% of analysed area) D50 and D90. An additional optical characterisation method is intended for polished ITER torus discs to identify non-diamond like phase inclusions and cracks. The detection of these defect structures with a microscope is performed by an automatical scale-up mapping in all spatial directions. Size and location of defects are the basis for the quality assurance.

KFM 14.10 Wed 16:00 Poster C

Ultra-cold neutron reflectivity and storage properties of ultra-nanocrystalline diamond films — •Hadwig Sternschulte[1,2], Andreas Frei[2], Peter Geltenbort[3], Christopher Geppert[4], Christian Gorges[4], Petra Müschenborn[2], Stefan Wenisch[2], Stephan Wlokka[2], and Nicolas Wöhrl[5] — [1]Hochschule Augsburg, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Kernchemie, Johannes Gutenberg-Universität Mainz, Germany — [5]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Ultra-cold neutrons (UCN) have kinetic energies of <300 neV and are used for high precision experiments such as the search for a non zero electrical dipole moment or an accurate determination of the neutron life time. To avoid disturbances the set-up is not located directly at the UCN source and the UCN are transported via total reflection from the source to the experiment. Diamond is an excellent reflector for UCN due to the high atom density in combination with a large bound coherent scattering length and low loss cross sections. Ultra-nanocrystalline diamond (UNCD) films with a very low surface roughness independent of the film thickness can be grown on various 3D shaped substrates by chemical vapour deposition. Therefore they are promising candidates for UCN reflecting layers. In this work we present studies of the UCN reflection and storage properties of UNCD thin films grown on planar 6" Si substrates. The influence of the UNCD film morphology and composition on the reflectivity and storage properties will be discussed.

KFM 14.11 Wed 16:00 Poster C

Abbility of hard metal tools coated with nanocrystalline CVD diamond films to machine ceramic materials — •Jakob Grau[1], Hadwig Sternschulte[1], Nicolas Wöhrl[2], Harald Leiste[3], Sven Ulrich[3], David Gholar[1], Björn Backes-Eckert[1], Achim Rösiger[1], Ralf Goller[1], and Doris Steinmüller-Nethl[4] — [1]Hochschule Augsburg, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [3]KIT, Institute for Applied Materials, Eggenstein-Leopoldshafen, Germany — [4]CarbonCompetence GmbH, Wattens, Austria

Ceramic materials including ceramic composite materials are hard and brittle materials difficult to machine. In principle, milling processes with defined cutting geometries are advantageous to machine materials due the higher removal rates. But hard metal tools do not withstand the abrasion caused by the ceramic material. Protective coatings such as thin nanocrystalline diamond films grown by chemical vapour deposition (CVD) allowing the conformal coating of defined milling tool geometries are an option to enhance the tool life time. In this work hard metal tools in four different geometries coated with nanocrystalline diamond films with measured sp^2/sp^3 C concentration, grain size and stress state were applied to machine C/C-SiC CMC consisting of carbon fibres with SiC as matrix. During the milling process the forces acting on the tool were recorded. It was found that it is in principle possible to machine CMC with CVD diamond coated tools. The influence of the tool geometry on the life time of the tool and especially on the mechanism of the failing process will be discussed.

KFM 14.12 Wed 16:00 Poster C

Effect of synthesis method on properties of multiferroic lead iron niobate — •Nicole Bartek, Vladimir Shvartsman, and Doru Lupascu — Institute for Materials Science and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany

Lead iron niobate, Pb(Fe0.5Nb0.5)O3 (PFN), belongs to multiferroics. That means that at least two types of ferroic order: ferroelectric and antiferromagnetic, coexist. Dielectric and magnetic properties have been studied in PFN powders, ceramics, and thin films, and the phase transitions from paraelectric (PE) to ferroelectric (FE) at around 380 K and from paramagnetic to antiferromagnetic states at around 140 K are well known. There is a certain scattering of data across literature, related to different methods of preparing PFN ceramics. Our work is focused on the synthesis and characterization of PFN ceramics via different methods and the comparison of their properties. Microstructure was analyzed by using X-ray diffraction and scanning electron microscopy. Electric properties and PE/FE phase transition were studied by dielectric spectroscopy and polarization hysteresis loop measurements. Magnetism and magnetoelectric properties were studied by vibrating sample magnetometry. Optical properties and band gap were investigated through Raman and UV-vis spectroscopy in dependence of temperature.

KFM 14.13 Wed 16:00 Poster C

Ba and Mn co-Doped Bismuth Ferrite ($BiFeO_3$) Nanoparticles: Tailoring the Multiferroic Features Through Phase

Transformation — •Astita Dubey, Marianela Escobar, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Multiferroic Bismuth Ferrite (BiFeO3; BFO) Nanoparticles (NPs) are noteworthy suitable materials for spintronics and memory devices due to their advantageous ferroelectromagnetic properties at room temperature. The research on BFO NPs is getting much attention due to enormous magnetic and photocatalytic behavior than their bulk counterparts. We reported systematic study of phase transition and impact on the multiferroic properties due to doping of Ba and Mn in pristine BFO NPs (BixBa1-xFeyMn1-yO3). Crystalline doped NPs sized 30-50 nm exhibit higher crystallographic symmetry from rhombohedral (R3c) to orthorhombic (Pbnm) with enhanced size induced magnetization as well as decrement in impure phases. All NPs were synthesized by wet chemical route (modified sol-gel and hydrothermal) and characterized via UV-VIS absorption spectroscopy, XRD diffraction, TEM, EDX, SEM, Impedance dielectric spectroscopy and Magnetic force microscopy.

KFM 14.14 Wed 16:00 Poster C

Substrate dependant crystalline phases of $TmFeO_3$ thin films — •Sven Becker, Mathias Kläui, and Gerhard Jakob — Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

$TmFeO_3$ (TFO) has orthorhombic structure in bulk and does not show ferroelectric polarization. S.-J. Ahn [1] has demonstrated that TFO grows in a hexagonal phase on Al_2O_3 substrates, which imposes mulitferroic properties. In this work we prepare TFO thin films on various substrates by pulsed laser deposition and observe both orthorhombic as well as hexagonal phase of TFO depending on the choice of substrate material. In a second step we evaluate the possibility to use TFO as a purely antiferromagnetic random access memory. Kosub [2] has shown this approach using Cr_2O_3. The antiferromagnetic state of multiferroic material is read out by anomalous hall effect in a platinum top layer. [1] S.-J. Ahn et al., J. Mater. Chem. C **4**, 4521(2014) [2] T. Kosub et al., Nat. Comm. **8**, 13985 (2017)

KFM 14.15 Wed 16:00 Poster C

Resistive switching of $La_{0.7}Sr_{0.3}MnO_3/PbZr_{0.2}Ti_{0.8}O_3$/Pt heterostructures — •Tino Band[1], Diana Rata[1], Robert Roth[1], Stefan G. Ebbinghaus[2], and Kathrin Dörr[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06099 Halle, Germany — [2]Institute of Chemistry, Martin Luther University Halle-Wittenberg, Kurt-Mothes-Straße 2, 06099 Halle, Germany

Electric fields in the order of 1-10 MV cm^{-1} are often applied at thin ferroelectric films to study electron tunneling through a barrier. An electric field of this magnitude can drive processes which are of electrochemical nature and change the chemical composition in or near the tunnel barrier. Until now, ferroelectric $PbZr_xTi_{1-x}O_3$ (PZT, x=0-0.5) has rarely been studied with respect to ionic-driven resistive switching. We present results on PZT films (x=0.2) grown on $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$(001) showing resistive switching like $SrTiO_3$. We have confirmed this for 3 nm thick PZT in nanoscale force microscopy measurements of current-voltage loops at fixed tip positions with subsequent detection of topographic changes. This experimental approach allows one to correlate ionic processes with the features of current-voltage characteristics. As second example, current-voltage characteristics of 10 nm thick PZT with $40\times40\,\mu m^2$ Pt top electrodes have been studied. Both types of measurements reveal resistive switching driven by ionic motion in large electric fields.

KFM 14.16 Wed 16:00 Poster C

Interplay of oxygen vacancies and conductance in $SrMnO_3$ ferroelectric domain walls — •Lokamani Lokamani[1], Peter Zahn[1], and Sibylle Gemming[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany

Strontium manganate ($SrMnO_3$), a perovskite polymorph, exhibits cubic structure at high 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 $SrMnO_3$ 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 retention times.

Here, we present a detailed first-principle investigation of the domain wall formation in strained $SrMnO_3$, the 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 will be presented.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)

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KFM 14.17 Wed 16:00 Poster C

Enhancing magnetoelectric coupling in 0-3 composite ceramics — •Doru C. Lupascu[1], Muhammad Naveed-Ul-Haq[1], Shvartsman Vladimir V.[1], Salamon Soma[2], Weber Samira[2], Wende Heiko[2], Labusch Matthias[3], and Schröder Jörg[3] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg- Essen, Universitatsstraße 15, 45141 Essen, Germany — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [3]Institute for Mechanics, Department of Civil Engineering, University of Duisburg-Essen, Universitatsstraße 15, 45141 Essen, Germany

It is well established that the highest magnetoelectric coupling can be achieved for systems that use a mechanical resonator at or near resonance typically realized as 2-2-layered devices of a magnetostrictive phase and a piezoelectric material. Statically, the coupling must, nevertheless, not be so high, because amplitude enhancement at high mechanical quality factor can be enormous. We show that statically also 0-3 composites show considerable coupling. It is in particular advantageous to seek for a material combination that uses not necessarily large absolute magnetostriction and electrostrictive strain, but rather places the system at external fields, where the largest changes of each arise. A very significant improvement of magnetoelectric coupling was achieved when combining NiFe2O4 with a relaxor ferroelectric system based on (Ba,Ca)(Zr,Ti)O3. [1] M. Naveed-Ul-Haq, et al., Acta Materialia 144 (2018) 305 - 313

KFM 14.18 Wed 16:00 Poster C

The K-edge of Hexagonal Boron Nitride Revisited: Effects of Electron-phonon Coupling on the Absorption Spectrum — •Ferenc Karsai[1], Moritz Humer[2], Georg Kresse[1,2], Espen Flage-Larsen[3], and Peter Blaha[4] — [1]VASP Software GmbH, Sensengasse 8, Vienna, Austria — [2]University of Vienna, Department of Physics, Sensengasse 8, Vienna, Austria — [3]SINTEF Materials and Chemistry, Oslo, Norway — [4]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, Vienna, Austria

The theoretical X-ray absorption near-edge structure for the boron and nitrogen K-edge in hexagonal boron nitride is investigated in great detail employing density-functional theory calculations. Electron-hole interactions are described using the super-cell core-hole method and the Bethe-Salpeter equation. The calculations are carried out with two different codes, the VASP and the WIEN2k code employing the projector augmented wave and the full-potential linear augmented plane-wave method, respectively. Close agreement between spectra obtained from the two codes is found. However, the boron spectrum obtained in the absence of vibrational effects shows significant deviations from experiment. Particularly the calculated spectrum yields a single 2p sigma peak and hence totally fails to describe the experimentally observed double-peak structure. By the inclusion of electron-phonon interactions the theoretical 2p sigma peak observes a significant splitting. We incorporate these effects in our calculations fully parameter-free and ab initio using a one-shot sampling method and obtain excellent agreement with experiment.

KFM 14.19 Wed 16:00 Poster C

Structural and many-body effects in the linear and nonlinear optical response of $KNbO_3$ from ab initio calculations — •Falko Schmidt, Arthur Riefer, Wolf Gero Schmidt, and Arno Schindlmayr — Universität Paderborn, Paderborn, Germany

Potassium niobate ($KNbO_3$), a perovskite-structure ferroelectric, is widely employed in nonlinear optical applications. Because of its small unit cell, $KNbO_3$ is ideally suited to assess the performance of *ab initio* computational methods for nonlinear optical materials that can be extended to related, more complex materials. After a careful structure optimization, we calculate the linear and nonlinear optical response of

$KNbO_3$ in the structurally simple cubic and tetragonal as well as the technologically important orthorhombic phase. While the Kohn-Sham band structure is corrected by *GW* self-energy shifts, excitonic effects are incorporated by solving the Bethe-Salpeter equation for the linear response. We find a strong dependence on the underlying atomic structure, especially for nonlinear optical spectra. The latter are also strongly affected by the band corrections from the *GW* approximation.

KFM 14.20 Wed 16:00 Poster C

Influence of quasiparticle and excitonic effects on the optical signatures of polarons and bipolarons in $LiNbO_3$ from *ab initio* calculations — •Falko Schmidt, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Germany

Lithium niobate ($LiNbO_3$), a perovskite-structure ferroelectric, is widely employed in nonlinear optical applications. A direct comparison between experiment and theory is difficult, however, as this material exhibits a large concentration of intrinsic defects, which strongly influence the optical properties. To reproduce the so-called polaron and bipolaron peaks found in the experimental measurements of the absorption spectrum, we test different possible defect types embedded in a supercell. Starting from density-functional theory, we correct the Kohn-Sham band structure by *GW* quasiparticle shifts, while excitonic effects are incorporated by solving the Bethe-Salpeter equation. The results shed light on the possible origin of the observed peaks due to the different optical characteristics of the investigated defects.

KFM 14.21 Wed 16:00 Poster C

Quasi particle energies and optical properties of $KTiOPO_4$ calculated by first principles — •Sergej Neufeld, Adriana Bocchini, Uwe Gerstmann, Arno Schindlmayr, and Wolf Gero Schmidt — Universität Paderborn

Potassium titanyl phosphate ($KTiOPO_4$, KTP) is a ferroelectric material that has been utilized in numerous applications based on non linear optics and photonics.
Despite its widespread use, many KPT properties are insufficiently understood. This concerns, e.g. its band gap. Earlier theoretical studies are based on the single-particle picture and report values between 3.0 - 4.0 eV.
In this work, quasiparticle and excitonic effects on the band structure and dielectric function of stoichiometric KTP are studies within the GW0 approximation and by solving the Bethe Salpeter equation (BSE), respectively. It is found that quasiparticle effects open up the band gap to about 5.3 eV. The solution of the BSE yields exciton binding energies of the order of 1.5 eV. Calculations that include both quasiparticle and excitonic effects are found to account for the measured reflectivity.

KFM 14.22 Wed 16:00 Poster C

Transient absorption in iron-doped lithium niobate induced via tailored optical excitation paths — •David Brinkmann, Simon Messerschmidt, Andreas Krampf, Laura Vittadello, and Mirco Imlau — School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany

Doping of lithium niobate (LN) with transition metals, e.g. iron, has a strong impact on the optical properties as well as transport dynamics of optically excited charge carriers. The most of these effects were investigated by the technique of light-induced absorption (LIA) and pump-wavelengths in the visible spectral range preferring a charge transfer from Fe^{2+} to Nb^{5+} (D-band). In this study, we present LIA data measured under three different, tailored experimental conditions, i.e., a combination of different iron concentrations and Fe^{2+}/Fe^{3+} ratios in the crystal and an excitation wavelength in the UV spectral range (355 nm), with the aim to excite the sample via a charge transfer from O^{2-} to Fe^{3+} (C-band) or O^{2-} to Nb^{5+} (LN band-edge). Our results demonstrate clearly the possibility to alter the induced absorption both in the spectral range and relaxation time by order of magnitudes as a function of the excitation paths. All of our observations can be explained straightforwardly by using the excitation and recombination model proposed by Messerschmidt *et al.* [J. Phys.: Condens. Matter (2018) doi: 10.1088/1361-648X/aaf4df] which is based on the presence of both, small polarons as well as self-trapped excitons trapped at different lattice positions. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.23 Wed 16:00 Poster C

Temperature-dependent fs-pulse-induced luminescence of lithium niobate — •Janina Ringel, Andreas Krampf, Simon Messerschmidt, and Mirco Imlau — School of Physics, Osnabrueck University, Barbarastr. 7, 49076 Osnabrueck, Germany

Temperature-dependent luminescence of lithium niobate (LN) after fs-pulse illumination is investigated over a large temperature range, i.e., from 10–300 K. As the luminescence intensity decreases exponentially above 100 K, a continuous broadening and shift of the peak position can be observed. Therefore, self-trapped excitons which are accounted for the low-temperature luminescence of LN (Blasse, Mat. Chem. Phys. **14**, 1986) are present at room temperature as well. However, above 200 K an unexpected deviation of the temperature-dependent emission peak from the well-known Varshni-behavior is found. Expressions based on phonon emission and absorption governed by Bose-Einstein statistical factors fail to describe the observed dependency of the peak position and halfwidth, as well (Viña, Phys. Rev. B **30** (4), 1984). We therefore discuss the presence of a second luminescing center.
Additional time-resolved luminescence data are presented. The decay time decreasing exponentially above 100 K limits the maximum temperature to 180 K. We show that a total of three different decay dynamics are present in heavily Mg-doped samples. Two of them, recently investigated (Kämpfe, Phys. Rev. B **93**, 2016), are lying in the μs–ms and second range, respectively. Here, both are observed for a larger temperature range. Financial support by the DFG (IM37/11-1, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.24 Wed 16:00 Poster C

Charge carrier dynamics in $SrTiO_{3-\delta}$ — •Thomas Schunk-Born[1], Christoph Grams[1], Kamran Behnia[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux (UMR 8213 CNRS-ESPCI), PSL Research University, Paris, France

Pristine $SrTiO_3$ is a quantum paraelectric insulator with a comparatively high permittivity of ∼300 already at room temperature. Upon cooling, its dielectric constant ε' shows a steep rise, usually indicative of a ferroelectric phase transition. In $SrTiO_3$, this transition is suppressed by quantum fluctuations and instead a saturation value of ε' of the order of 10^4 is observed [1].

By reducing the oxygen content, charge carriers are introduced in $SrTiO_{3-\delta}$. Due to the large effective Bohr radius caused by the high permittivity, the material becomes conducting and even superconducting at unusually low charge carrier densities [2].

Using broadband dielectric spectroscopy, we investigate the conductivity of samples with different charge carrier densities depending on frequency and temperature to show an evolution from insulating ($\sigma' \approx 0$), to variable-range-hopping ($\sigma' \propto \omega^s$), to Drude-metal ($\sigma' \propto \omega^{-2}$) behavior.

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[1] R. Viana *et al.*, Phys. Rev. B **50**, 601 (1994)
[2] X. Lin *et al.*, Phys. Rev. X **3**, 021002 (2013)

KFM 14.25 Wed 16:00 Poster C

Time-resolved multicolor emission of harmonic nanoparticles via nonlinear frequency mixing — •Jan Klenen[1], Christian Kijatkin[1,2], Bjoern Bourdon[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

Harmonic nanoparticles (HNPs) attract growing interest owing to their unique nonlinear optical (NLO) properties such as loosened phase-matching conditions. Motivated by applications in the fields of multiphoton microscopy and holography, thorough investigations on harmonic generation have been sparked. Nevertheless, reports on three-wave mixing processes in HNPs are scarce, especially with respect to temporal evolution, even though this approach may pave the way towards ultrafast sub-ps time-resolved microscopy and fluorescence upconversion spectroscopy (FLUPS). Using two nondegenerate femtosecond pulses, transient nonlinear frequency mixing (FM) processes are studied comprehensively in nanoscaled lithium niobate powder plaques and thin particle layers using NLO diffuse reflectometry [C. Kijatkin *et al.*, *Photonics* **2017**, *4*(1), 11]. A particular focus is given to the spectrotemporal analysis of multicolor emission exceeding the visible spectral range. Further assessment is performed in regard to FLUPS through upconversion of a picosecond pulse in order to test the viability of HNP powders as an alternative to crystalline media as a flexible material for different scalings and wavelengths. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 14.26 Wed 16:00 Poster C

Investigation of an inline detection system for conversion coatings on aluminum alloys by means of specular reflectance — •Yannic Toschke[1], Jörg Rischmüller[1], Mirco Imlau[1], Simon Podendorf[1], Mareike Schlag[2], Kai Brune[2], and Hauke Brüning[2] — [1]School of Physics, Osnabrueck University, Barbarastraße 7, 49076 Osnabrueck, Germany — [2]Fraunhofer IFAM, Wiener Strasse 12, 28359 Bremen, Germany

In accordance with Europe*s REACH agreements 2017 (Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals) restrictions of conversion coatings for metallic surfaces containing Cr^{+6} have further led to investigations of suitable alternatives. Reasoning behind those restrictions were the confirmed carcinogenic properties of hexavalent Chromium. One possible approach comparable in its corrosion inhibition and function as adhesion agent consists of Cr^{+3} and Zr^{+4}. Precise control of the process parameters is crucial for the performance of any kind of coating. Therefore, an additional method for inline quality control is desired. In this study a reliable and non-destructive method based on specular reflectance will be discussed matching those requirements. Five different qualities of the given conversion coat (20-70 nm) were applied on two different aluminum alloys (AA3003 and AA6060) and investigated with REM, LIBS and corrosion tests. Differentiation between each coating and the uncoated substrate are shown. Correlation between the gathered measurements suggests that an affordable method for inline quality control was found. Prime influence seems to arise from the morphology of the coating.

KFM 14.27 Wed 16:00 Poster C

Zone-plate based soft X-ray microscopy with sub-10 nm resolution — Rainer H. Fink[1,2], Joshua Loroña Ornelas[1], •Andreas Späth[1], Jörg Raabe[3], Christian David[3], and Benedikt Rösner[3] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]CENEM, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland

Soft X-ray scanning transmission microspectroscopy (STXM) using Fresnel zone plates (FZPs) as focusing elements has developed into a routine technique for the investigation of semi-transparent thin film specimens. Routine operation of STXMs uses spatial resolution of around 30 nm, determined by the outermost zone width of the FZP. An elegant method to fabricate high-resolution FZPs has been introduced by doubling the line density obtained from the lithography step utilizing atomic layer deposition (ALD). We have recently prepared FZPs with line structures to about 7 nm, thus pushing the resolution limits into the sub-10 nm regime. We will report on the resolution tests of specific test samples, but also on technologically relevant specimens where the improvement in lateral resolution becomes inevitable. Determination of the spatial resolution was conducted using a two-dimensional Fourier shell correlation of two independent data sets. This yielded a real space resolution of < 8 nm considering the half-bit criterion. The project achieved funding by the BMBF (project 05K16WED), within the EU-H2020 Research and Innovation Programme, No. 654360 NFFA-Europe, and by Marie Skłodowska-Curie grant No. 701647.

KFM 14.28 Wed 16:00 Poster C

Efficient Iterative Phase Reconstruction for X-Ray Near Field Holography — •Johannes Hagemann[1], Silja Flenner[2], and Imke Greving[2] — [1]DESY, Notkestraße 85, 22607 Hamburg — [2]HZG, Notkestraße 85, 22607 Hamburg

An iterative solver has always a drawback compared to a single step solution: it takes more time to compute. For large data sets as they occur for example in x-ray propagation-based phase-contrast tomography, this can be a hindering factor. On the other hand an iterative scheme can be the only way to get a meaningful reconstruction of the object under survey [1].

In this contribution we demonstrate an algorithmic improvements on the alternating projection algorithm for better convergence. With this algorithm we were able to recover the phases of a strongly phase shifting and absorbing multi material specimen. This specimen has been ivory which was partly coated with Gallium during the FIB preparation process for the measurement. The measurements were obtained at the nano-imaging endstation of beamline P05 at PETRA III, DESY.

[1] J. Hagemann, M. Töpperwien and T. Salditt, "Phase retrieval for near-field X-ray imaging beyond linearisation or compact support," Appl. Phys. Lett., 113 (2018)

KFM 14.29 Wed 16:00 Poster C

μ lenses in Silicon Carbide — •Fiammetta Sardi — 3 pysics institute, Stuttgart, Germany

Silicon carbide(SiC) is an appealing material due to its properties in the applications of quantum technologies. Its wide-band gap and highly developed fabrication techniques show great potential as a resource in quantum technology evolution.

Silicon Vacancy Defects hosted in the crystalline structure of SiC exhibit a long relaxation time at room temperature and a manageable coherence control on a single spin. Nevertheless, the high refractive index of the material leads to strong refraction and total internal reflection ending in deviation of the defects* photoluminescence at SiC-air interface.

A possibility to decrease this effect is the fabrication of shallow Solid immersion lenses (SIL) of a few micrometres in size on a SiC wafer, resulting in refractionless transmission of light along the SIL surface. Defects are supposed to be placed in the centre of the SIL for maximum enhancement of collected photoluminescence .

In this work, a scalable method for the fabrication for SILs in SIC is presented, using photo-lithography and reaction ion etching(RIE) to transfer SILs from the photoresist to SiC. For lenses with an NA=0.7, enhancements higher than 2.5 in the photoluminescence of defects has been achieved.

KFM 14.30 Wed 16:00 Poster C

On the effect of high current densities on thin iron-carbon alloy films — •Thomas Brede, Christine Borchers, Reiner Kirchheim, and Cynthia Volkert — Institut für Materialphysik, Georg-August-Universität, Göttingen, Deutschland

The recently discovered flash sintering method for preparing high quality oxide materials can be applied to the preparation of high performance nanocrystalline metals as well. Just as for the oxide materials, it is possible to use electric fields and currents to enhance densification of metal powders while limiting grain growth, however, the exact mechanism is still under discussion. The goal of our study is to understand how electric currents effect impurity redistribution and grain growth in fine grained metals.

Thin nanocrystalline iron films with high carbon concentrations are prepared as a model system and to compare with the behavior of nanocrystalline bulk samples. The thin film samples are heated and exposed to high current densities comparable to those experienced during the sintering process of bulk materials and the evolution of the microstructure, morphology and carbon concentration are investigated using electron microscopy. Extensive effects of the electrical current on C redistribution and grain growth are observed, including strong coupling between grain growth and C content and the formation of grains that are elongated along the direction of the current. The various microstructural observations will be summarized and possible explanations will be discussed.

KFM 14.31 Wed 16:00 Poster C

Mask-less, high aspect ratio, high resolution electron-beam-induced etching of diamond — •Vasilis Dergianlis, Martin Geller, Dennis Oing, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Diamond has attracted significant attention as a promising material for a broad range of emerging applications, such as host material for NV-centers in future quantum information technologies [1], or as ultrasensitive nano-sensors [2]. Structuring this extremely stable material is, however, highly challenging. First attempts have shown the possibility to use water vapor in combination with an electron beam [3], however only with a strong anisotropy of the etching process and a low-resolution in the μm-range.

In this contribution, we report on high-resolution etching of undoped, hydrogen-terminated, single crystalline diamond layers of <100> orientation without anisotropy in the etching process. We used a Scanning Electron Microscope (SEM) in a dual beam Focused Ion Beam (FIB) together with water vapor, which was injected directly onto the sample surface. Using this versatile and non-invasive technique, trenches with widths of only 10 nm were precisely etched into the diamond sample. Our results show the possibility of high-resolution mask- and resistless patterning of diamond for nano-optical and electronic applications.

[1] Dutt et al., Science **316**, 1312 (2007)
[2] Maze et al., Nature **455**, 644 (2008)
[3] Martin et al., Phys. Rev. Lett. **115**, 255501 (2015)

KFM 14.32 Wed 16:00 Poster C

Improved automatic proton beam writing — •Lukas Jäger, Alrik Stegmaier, and Hans Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen Germany

Proton beam writing is a maskless lithographic technique using a focused high energy proton beam to pattern materials and create high aspect-ratio 3D structures. At the II. Institute of the University Göttingen a tandem accelerator with a beam line for proton beam writing is available. To control the beams position on the sample, the sample-holder can be moved by two piezo stages. First the beam shape is measured via a PIXE measurement on a Ni-grid. The beam shape can be used by a program to compute the near optimal movement of the sample-holder during irradiation. Instead of rasterizing the desired pattern, the program optimizes the irradiation pattern to enable the irradiation of more complex patterns. Recent advances in the software development improved stability, fail safety and accuracy of the irradiation process, including a newly automatic blanking system.

KFM 14.33 Wed 16:00 Poster C

Cu-poor region of the CuI phase diagram: An ab initio study — •Stefan Jaschik, Mário Rui Gonçalves Marques, and Miguel A. L. Marques — Institut für Physik, Martin-Luther-Universität, Halle-Wittenberg, D-06099 Halle (Saale), Germany

We studied the Cu-poor region of the phase diagram of CuI using both global structural prediction methods and cluster expansion techniques. We found that, at the level of the Perdew-Burke-Ernzerhof approximation to the exchange-correlation functional, there are ordered-defect compounds that are energetically favored with respect to pristine CuI. This may explain the large number of Cu vacancies that is usually found in experimental samples.

KFM 14.34 Wed 16:00 Poster C

Small bound polarons in $LiTaO_3$ — •Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen

The optical response of many oxide crystals including the electro-optic material $LiNbO_3$ has been successfully explained by the presence of small polarons. The latter are quasiparticles formed when the interaction of a charge carrier with the surrounding lattice is strong enough to trap the charge carrier at essentially one lattice site. While different kind of small polarons have been described [1] and demonstrated [2] in $LiNbO_3$, much less is known concerning the isomorphic and isoelectronic $LiTaO_3$. Although the existence of small bound polarons might be expected due to the high lattice polarizability, the verification of this assumption is still missing. In this work we provide the atomistic description of small bound polarons $Ta_{Li}^{5+/4+}$ in $LiTaO_3$. The calculations performed within density functional theory with Hubbard corrections predict the large lattice relaxation of the oxygen ligands associated to the electronic capture at the antisite center, which can be interpreted as due to the polaron formation. The charge distribution is localized within essentially one unit cell and resembles the atomic Fe d_{z^2} orbitals, suggesting a scarce hybridization the Ta d orbitals.

[1] O. F. Schirmer et al., J. Phys.: Condens. Matter 21, 123201 (2009). [2] F. Freytag et al., Nature Scientific Reports 6, 36929 (2016).

KFM 14.35 Wed 16:00 Poster C

Plastic deformation in polycrystalline $BaTiO_3$ — •Marion Höfling[1], Pengrong Ren[2], Stefan Lauterbach[1], Xijie Jiang[1], Jurij Koruza[1], Till Frömling[1], and Jürgen Rödel[1] — [1]Department of Earth and Materials Science, Technische Universität Darmstadt, 64287 Darmstadt — [2]School of Materials Science and Engineering, Xi'an University of Technology, Xi'an, P.R. China

Oxides can exhibit dislocations with charged cores and charge-compensating surrounding layers. These dislocations are in general considerably more temperature stable than point defects and have been described as one-dimensional dopants. Some recent publications have demonstrated that changing the dislocation density can be used to tune individual material's properties, for example the ionic conductivity in TiO2 [1]. In this study we investigated the plastic deformation of polycrystalline BaTiO3 as a possible means to introduce dislocations into ceramics. The creep mechanisms of BaTiO3 were determined at different temperatures and stresses based on the power law exponents obtained from high-temperature uniaxial compression experiments and a first approximation for a deformation mechanism map was created. Several samples were successfully plastically deformed on the border of the diffusion-dislocation creep regime and the resulting effects on the ferroelectric and dielectric properties were examined. Transmission electron microscopy (TEM) and piezo force microscopy (PFM) were carried out to identify the influence of the creep experiments on the microstructure and the domain evolution.

[1] Adepalli et al. Phys. Chem. Chem. Phys., 2014, 16, 4942

KFM 14.36 Wed 16:00 Poster C

Pressure-induced amorphization of dynamically compressed and heated minerals by X-ray diffraction and electron microscopy — •Christoph Otzen[1], Hanns-Peter Liermann[1], and Falko Langenhorst[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institut für Geowissenschaften, Jena, Germany

Large planetary meteorite/asteroid impacts play a crucial role in the history of the Earth, traces of which can still be found in minerals today and provide important information about past impact events. The most significant impact indicator is the amorphization of many minerals and many studies have been performed to constrain the conditions for amorphization as a function of pressure and compression rate. The effects of temperature and grain sizes, however, have not yet been investigated accurately and *in-situ*, due to experimental limitations and the extreme conditions attained during shock compression.

In this study, we carried out dynamic compression experiments and simultaneously measured *in-situ* X-ray powder diffraction of abundant rock-forming minerals. We use membrane-driven diamond-anvil cells to rapidly compress the samples to high pressures and are in the process of developing a new setup for simultaneous pressure and temperature increase. We aim at creating the thermodynamic conditions that can be found in natural impacts in an effort to constrain the conditions for amorphization more precisely. We will present initial results of these diffraction experiments and the analyses on the recovered samples by transmission electron microscopy.