DF 16: Crystallography - Poster Session (KR with DF)

Time: Wednesday 18:00–20:00 Location: P4

DF 16.1 Wed 18:00 P4

Structural and magneto-electric investigations of Erythrosiderites — •Tobias Fröhlich[1], Daniel Brüning[1], Ladislav Bohatý[2], Petra Becker[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Most erythrosiderites of the form $A_2[FeX_5(H_2O)]$ are magneto-electric without multiferroicity. However, in 2013 it was found that the compound $(NH_4)_2[FeCl_5(H_2O)]$ is multiferroic. A comparison of macroscopic and microscopic properties of different compounds of this family reveals interesting insights into the structural order and magnetic coupling. While the crystal structures of most erythrosiderites can be described with space group *Pnma*, $Cs_2[FeCl_5(H_2O)]$ has space group *Cmcm*. In contrast to the other compounds [1, 2], its magnetic structure is not yet directly determined. However, there are investigations of macroscopic quantities, which allow to predict the magnetic structure [3]. We present a neutron study of the magnetic structure of $Cs_2[FeCl_5(H_2O)]$, which perfectly explains these measurements. Furthermore, $Cs_2[FeCl_5(H_2O)]$ exhibits a structural phase transition which was discovered in 1987 [4]. By single crystal X-ray diffraction, we solved the structural distortion associated with this transition, which involves a slight monoclinic distortion into space group $C2/c$.

[1] M. Gabás et al. (1995), J. Phys. Condens. Matter **7** 4725-4738 [2] J. Rodrígues-Velamazán, et al. (2015), arXiv [3] M. Ackermann et al. (2014), J. Phys. Condens. Matter **26** 506002 [4] J. Chadwick et al. (1987), J. Phys. C: Solid State Phys. **20** 3979-3983

DF 16.2 Wed 18:00 P4

Investigation of new phases in the Ba-Si phase diagram under high pressure by ab initio structural search — •Jingming Shi[1], Wenwen Cui[1], José Flores-Livas[2], Alfonso San-Miguel[1], Silvana Botti[3,1], and Miguel Marques[4,1] — [1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France — [2]Department of Physics, Universität Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Barium silicides are versatile materials that have attracted attention for a variety of applications in electronics and optoelectronics. Using an unbiased structural search based on a particle-swarm optimization algorithm combined with density functional theory calculations, we investigate systematically the ground-state phase stability and structural diversity of Ba–Si binaries under high pressure. The phase diagram turns out to be quite intricate, with several compositions stabilizing/destabilizing as a function of pressure. In particular, we identify novel phases of BaSi, $BaSi_2$, $BaSi_3$, and $BaSi_5$ that might be synthesizable experimentally over a wide range of pressures. Our results not only clarify and complete the previously known structural phase diagram, but also provide new insights for understanding the Ba–Si binary system.

DF 16.3 Wed 18:00 P4

Watching the Verwey transition of Magnetite by Timeresolved X-Ray diffraction — •Alexander von Reppert[1], Jan-Etienne Pudell[1], Flavio Zamponi[1], Azize Koc[2], Stephan Geprägs[3], Jose Emilio Lorenzo[4], Luc Ortega[5], Matthias Reinhardt[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz-Zentrum Berlin BESSY II, Albert-Einstein Str. 15, 12489 Berlin, Germany — [3]Walther-Meißner-Institut, Bayerische Akademie d. Wissenschaften, 85748 Garching, Germany — [4]Institut Nèel, CNRS & Univ. Grenoble Alpes, 38042 Grenoble, France — [5]Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France

We present timeresolved X-Ray diffraction from a 300 nm thin Magnetite(Fe3O4) film that is driven across the Verwey transition by fs-laser excitation. The prototypical insulator to metal transition at 123 K is accompanied by a peak intensity increase and peak width decrease of structural Bragg peaks, which we attribute to the destruction of trimerons that lead to inhomogeneous lattice strain in the low T phase. Our systematic investigations of the lattice dynamics yield two timescales: An ultrafast peak width drop - probably due to electronic processes - which is subsequently enhanced by transport and equilibration of the excitations. Complementary to our lab-based Plasma X-Ray source we conducted measurements at the XPP beamline at the synchrotron BESSY II where we observe that the recovery timescale depends crucially on the proximity to the transition temperature.

DF 16.4 Wed 18:00 P4

Detection of pressure and density waves (acustic waves) in liquid crystal near the phase transition temperature by gold nano particle — •Ricardo Rose, Andre Heber und Frank Cichos — Universität Leipzig Fakultät für Physik und Geowissenschaften, Leipzig, Germany

Recent studies have shown, that the intensity of a polarized laser beam can be modulated by a second heating laser beam, which excites plasmons on gold nanoparticles (AuNp) positioned in liquid crystal (LC). The exited AuNp dissipate the energy as heat into the LC. If the LC is near below the phase transition point from nematic phase to isotropic phase, the dissipated heat will suffice to build an isotropic bubble around the AuNp. The size of the bubble can be controlled by the amount of supplied energy. While the polarization within the nematic phase is rotated due to different refractive indices for the ordinary and extraordinary axis similar to a $\lambda/2$ - plate, the polarization will be conserved within the isotropic phase. If an analyzer is placed behind the LC, the intensity of the probe laser beam can be modulated by the optical path length within the nematic phase and their disturbance within the isotropic bubble around the laser heated AuNp. In this study we investigate, if the deformation of the isotropic bubble by acoustical waves and the linked modulation of the probe laser beam intensity at constant, unmodulated power of the heating laser will be clearly detectable, while the ambient temperature is near the phase transition temperature. If that can be proven, we will able to design a microphone at nano size.

DF 16.5 Wed 18:00 P4

Ga^{3+} Substitution in the Brownmillerite-Type Phase $Ca_2Fe_2O_5$: Structural and Spectroscopic Investigations — •Quirin Stahl[1,2], Andreas Reyer[1], Reinhard Wagner[1], Gerold Tippelt[1], and Günther J. Redhammer[1] — [1]Department Chemistry and Physics of Materials, University of Salzburg, Austria — [2]Institute of Structural Physics, Technische Universität Dresden

Brownmillerite-type compounds with the general formula $A_2B'_{2-x}B_xO_5$, where A = alkaline earth metals and B'/B = group III or transition-metal atoms, are among the most frequently studied oxygen-deficient perovskites. 61 synthetic single-crystal samples of $Ca_2Fe_{2-x}Ga_xO_5$ with $0.00 \leq x \leq 1.328$ have been investigated by single-crystal X-ray diffraction at RT. We find that pure $Ca_2Fe_2O_5$ and samples up to x = 0.989 have space group *Pnma*, Z = 4, whereas samples with x > 0.989 show *I2mb* symmetry, Z = 4. We also performed a detailed Raman study of Ga^{3+} and Al^{3+} doped $Ca_2Fe_2O_5$. The polarized Raman measurements of $Ca_2Fe_{2-x}Ga_xO_5$ single-crystals enable us to assign eleven of the thirteen theoretically predicted A_g modes. Furthermore the change from *Pnma* to *I2mb* space group symmetry is reflected by a significant change of two Raman modes below 150 cm^{-1}. These Raman modes are obviously linked to changes of the Ca-O bond lengths at the phase transition. To complete the study of the $Ca_2Fe_{2-x}Ga_xO_5$ series, we have performed a detailed Mössbauer spectroscopic study as a function of the chemical composition, mainly to fix site occupation number by a second, independent method beside XRD.

DF 16.6 Wed 18:00 P4

Synthesis and controlled growth of α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT) — •Martin Grönke, Mihai-Ionut Sturza, Barbara Eichler, Sandra Schiemenz, Victoria Eckert, Silke Hampel, and Bernd Büchner — IFW Dresden

Crystal growth of different transition metal halogenides representing a very up to date research topic in solid state chemistry surface physics. Among the interest for materials with strong anisotropic bonding-dependent interactions, resulting frustration effects could stabilize new patterns of cooperative magnetic interactions, or even a spin-liquid-

state. One candidate to realize a Kitaev spin model is the layered honeycomb magnet α-Rutheniumchloride (α-RuCl3) with strongly frustrated, anisotropic interactions between spin-orbit entangled jeff = 1/2 Ru3+ magnetic moments.

Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. Herein we present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT). To understand the growth mechanisms and to optimize the synthesis we performed thermodynamic modelling with the program Tragmin. We obtained very thin single crystals by CVT with heights around 40 nm. The crystal habit is characterized by means of SEM, TEM and AFM. Furthermore EDX, WDX, XRD, micro-RAMAN and SQUID-VSM measurements proving composition, phase-purity and predicted magnetic properties.