Dear participant,

Welcome to the 35th International Symposium on Dynamical Properties of Solids - DyProSo XXXV - which is held from 13 to 17 September 2015 at the Bildungszentrum Freising near Munich. The conference is hosted by the Heinz Maier-Leibnitz Zentrum (MLZ) for neutron research (www.mlz-garching.de).

DyProSo is a 4-day research meeting aiming at the promotion of new ideas and concepts concerning functional properties of condensed matter by stimulating scientific discussions between young and experienced scientists actively working on dynamic properties of materials.

The scientific programme of DyProSoXXXV focuses on:

- Amorphous and Soft Matter
- Multiferroics and ferroelectrics
- Electrons and spins
- Diffusive dynamics
- Phonons and magnons
- Theoretical and experimental methods
- Excitations of strongly correlated electron systems
- Two-dimensional systems
- Materials under high pressure

There are 15 invited lectures, 30 contributed talks and 18 poster presentations. Following the traditions of DyProSo there are no parallel sessions.

It would be a great pleasure if you could join us from the very beginning on Sunday evening. As a warm-up there will be a welcome reception, courtesy of NUKEM Isotopes. Further social highlights are the guided tour through FRM II and the sight-seeing tour including the Cathedral and the Prince Bishop’s Residence. You are cordially invited to attend the conference dinner at the Bräustüberl Restaurant located at the Weihenstephan Hill. It belongs to the so called Oldest Brewery of the World “Weihenstephan” which has a close relationship to TUM.

I am very pleased to welcome you at the Bildungszentrum Freising and I wish you all and a pleasant stay in one of the oldest towns in Bavaria.

Winfried Petry (Conference chairman)
Contents

Venue .................................................. 8
Previous DyProSo conferences ................. 9
DyProSo committees ................................ 10
Sponsors ............................................... 11

Amorphous and Soft Matter

Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses ................................. 13
Boson peak in two liquid crystal glass-formers – results of the neutron scattering ....................... 15
Immense elastic softening and the responsible molecular mechanisms near the demixing phase transition of thermo-responsive polymer solutions ........................................... 17
Light-Controlled Topological Charge in a Nematic Liquid Crystal ............................................... 19

Multiferroics and ferroelectrics

High resolution polarized Raman scattering study of multiferroic MnWO4 ........................................ 21
Néel-type Skyrmion Lattice in a Polar Magnetic Semiconductor ..................................................... 23
Magnetic and orbital excitations in the multiferroic skyrmion host GaV₄S₈ ........................................... 25
Magnetic and magnetoelectric excitations in hexagonal multiferroics RMnO₃ probed by neutron scattering and THz spectroscopy ................................................................. 27
Probing ferroelectricity and magnetoelectric effect in RMnO₃ (R = Tb, Dy) by Fe³⁺ B-site substitution ................................................................. 29

Electrons and spins

Slow dynamics in magnetic pyrochlore oxide systems ..................................................................... 31
Probing the Dynamical Properties of Nanoscale Solid-State Systems in Real Space and Real Time .................................................................................................................... 33
Domain wall dynamics, local diffusion, and phonons in a lead-free relaxor ferroelectric ................. 35

Diffusive dynamics

Metal borohydrides: from hydrogen storage to electrochemistry ...................................................... 37
Heterogeneous dynamics in a Au-Si liquid investigated with quasielastic neutron scattering ......... 39
Shining light on atomic hopping processes - diffusion mechanisms in B2 alloys ............................ 41
Surface friction investigated by neutron scattering ............................................................................. 43

Phonons and magnons

Computation, the Gibbs Free Energy, and Inelastic Scattering ......................................................... 45
Phonons and magnetism in FeSi ........................................................................................................ 47
Ab Initio Computation of Phonon-Phonon and Magnon-Phonon Interactions: Successes and Challenges ................................................................. 49
Pretransitional dynamics in prototype antiferroelectric material PbZrO₃ ........................................... 51

Theoretical and experimental methods

Polarized Raman Spectra of Perovskite Relaxor Ferroelectrics ...................................................... 53

Excitations of strongly correlated electron systems

Electronic Raman Scattering in Cuprate Superconductors: The Pseudogap Story ........................... 55
New insights on the cuprates phase diagram from x-ray scattering .................................................. 57
Magnetic resonant excitations in S-doped iron-chalcogenide superconductors ................................ 59
Experimental and theoretical studies of the lattice dynamics in superconducting BaNi₂(As₁₋ₓPₓ)₂ .......................... 61
Charge order and superconductivity in the cuprates ........................................................................ 63
Excitonic effects on the optical response of quasi-one-dimensional Ta₂NiSe₅ and Ta₂NiS₅ ............. 65

Phonons and magnons

Inelastic scattering study of AgCrSe₂ ............................................................................................. 67
“Half-moon” excitations in the magneto-elastic spin liquid Tb₂Ti₂O₇ .................................................. 69
Temperature dependence and linewidths of Al phonon dispersions ............................................ 71
Theoretical and experimental methods

Dynamic properties of liquids and solids probed by Dynamic Mechanical Analysis 73
Non-exponential relaxation: multiscale or nonlinear phenomenon? 75

Two-dimensional systems

Structural and magnetic correlations in emergent materials 77
Theory of Piezoelectricity and Sound Waves in 2D Crystals 79
High Precision MC/RG Study of Elastic Fluctuations in Solid Membranes 81
Spectroscopical characterisation of high surface area carbons through a multitechnique approach 83

Materials under high pressure

(De)formation of mantle minerals: Insights from atomic-scale simulations 85
Lattice dynamics and magnetic order in CrAs under pressure 87

Multiferroics and ferroelectrics

Soft-mode spectroscopy of ferroelectrics and multiferroics 89
The nature of phase transition in GeTe - the parent compound of the phase-change materials 91
Directional anisotropy of light in multiferroics 93
Tiny cause with huge impact: polar instability through strong magneto-electric-elastic coupling in bulk EuTiO3 95
Multiferroic RMnO3 (R = Y, Tb, Ho) and isotopically substituted TbMn16/18O3, Dy16/18MnO3: A comprehensive Raman light scattering and neutron scattering investigation 97
Dynamics of Nanoscale Polarization Fluctuations in a Uniaxial Relaxor 99
Broadband Dielectric Spectroscopy of A-site Substituted Relaxor Ceramics 101

Poster session

Ab initio vibrational properties of the MXene materials functionalized by fluorine, oxygen and hydroxyl group 103
Reflection, refraction, mode conversion and guided waves on surfaces and interfaces of materials with all allowed Poisson ratios 105
Effects of 18O isotope substitution in multiferroic RMnO3 (R=Tb, Dy) 107
EPR Spectroscopy of Manganese-Doped Perovskite-Type Metal-Organic Framework 109
Low-energy lattice dynamics of relaxor-like PFN-38 %PT by inelastic neutron scattering 111
Elastic constants in multiferroic Bi2Mn4O10 113
Analytic approach to anharmonic modes of lattice vibrations 115
Effect of CFO and PZT fillers on Dielectric and Ultrasonic Properties of P(VDF-TrFE) Copolymer Based Composites 117
Order by disorder or energetic selection of the ground state in the XY pyrochlore antiferromagnet Er7Ti12O32: A neutron scattering study 119
Guided surface waves on interfaces of media with positive and negative Poisson's ratio 121
Electric control of the unidirectional transmission in the ferrotoroidic LiCoPO4 123
Dynamics of water confined in chrysotile asbestos studied by inelastic neutron scattering 125
Broadband dielectric response of polyaniline pellets as nanocomposites of metallic emeraldine salt and dielectric base 127
Directional dichroism at the spin-wave excitations of multiferroic Ni3TeO6 129
Ab initio study of the strain-mode coupling in SrBi2Nb2O9 131
Evolution of the helimagnon dispersion 133
New multiferroic materials on the base of Co-doped barium titanate 135
PANDA – the first cold TAS with overlap to thermal wavelengths 137

Index 138

List of participants 142

Map of Freising 149

Imprint 147
Venue

Bildungszentrum Freising – Kardinal-Döpfner-Haus
Domberg 27
85354 Freising
Phone: 08161/181-0
Fax: 08161/181 2850

Conference telephone
from Sunday, 13 September 4 pm throughout the conference:
+49 160-96939110

Previous DyProSo conferences

1. 1967 Albe, France
2. 1968 Oberwolbach, Germany
3. 1969 Mont Saint-Odile Nancy, France
4. 1970 Oberwolbach, Germany
5. 1971 Edinburgh, UK
6. 1972 Montpellier (Mont Aigoual), France
7. 1973 Leoni (Starnberger See), Germany
8. 1974 Giswil, Switzerland
9. 1975 Pelvoux, France
10. 1976 Reading, UK
11. 1977 Phonon Conference in Paris, France
12. 1978 Stresa, Italy
13. 1979 Ferroelectricity Conference in Edinburgh, UK
14. 1980 Le Houches, France
15. 1981 Überlingen, Germany
16. 1982 San Miniato, Italy
17. 1983 Leuven, Belgium
18. 1984 Mürren, Switzerland
19. 1985 Phonon Conference in Budapest, Hungary
20. 1986 Überlingen, Germany
21. 1987 Ventron, France
22. 1988 Sestri, Cinque Terri, Italy
23. 1989 Phonon Conference in Heidelberg, Germany
24. 1990 Chexbres, Switzerland
25. 1991 Autrans, France
26. 1992 Schellerau (Dresden), Germany
27. 1993 Lunteren, The Netherlands
28. 1994 Il Ciocco, Italy
29. 1995 Haro (Bilbao), Spain
30. 1996 (Crete, Greece - cancelled)
31. 1997 Davos, Switzerland
32. 1999 Tours, France
33. 2001 Kerkrade, The Netherlands
34. 2003 Trieste, Italy
35. 2005 Ceský Krumlov, Czech Republic
36. 2007 Porto, Portugal
37. 2009 Antwerp, Belgium
38. 2011 Aussois, France
39. 2013 Vienna, Austria
DyProSo committees

Conference Chairman:
• W. Petry, Scientific Director of Heinz Maier-Leibnitz Zentrum (MLZ) and the Research Neutron Source FRM II, Technische Universität München

International Advisory Board:
• A. Almeida, University of Porto, Portugal
• M.A. Carpenter, University of Cambridge, UK
• C. Ecolivet, CNRS, GMCM, University of Rennes, France
• I. Etxebarria, University of the Basque County, Bilbao, Espagne
• M. Fiebig, ETH Zürich, Switzerland
• J. Hlinka, Institute of Physics, Prague, Czech Republic
• T. Janssen, University of Nijmegen, The Netherlands
• M. Krisch, ESRF Grenoble, France
• J. Kulda, ILL Grenoble, France
• B. Partoens, University of Antwerp, Belgium
• S. Petit, LLB Saclay, France
• W. Schranz, University of Vienna, Austria
• S. Speziale, GFZ Potsdam, Germany
• C. Thomsen, TU Berlin Germany
• R. Torre, LENS, Florence, Italy
• P. Zieliński, Polish Academy of Sciences, Institute of Nuclear Physics, Poland

Program Committee:
• P. Böni, Physics Department, Technische Universität München, Germany
• G. Eckold, Institute for Physical Chemistry, University of Göttingen, Germany
• R. Hackl, Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften München, Germany
• Th. Keller, Max-Planck-Institut für Festkörperforschung, Germany
• M. Leitner, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) and Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Germany
• W. Petry, FRM II and MLZ, TUM, Germany
• W. Schranz, University of Vienna, Austria
• P. Zieliński, Polish Academy of Sciences, Institute of Nuclear Physics, Poland

Local Organizing Committee at MLZ/FRM II:
• W. Petry
• J. Neuhaus
• E. Jörg-Müller
• M. Leitner
• P. Neibecker
• B. Pedersen
• S. Valentin-Hantschel

Sponsors

We gratefully acknowledge the support of the Deutsche Forschungsgemeinschaft und NUKEM Isotopes.
Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses

CHUMAKOV, Aleksandr

European Synchrotron Radiation Facility (ESRF), Grenoble, France

Corresponding Author: chumakov@esrf.fr

The heat capacity of glasses at temperatures of about ~10 K for a long time was considered to be anomalously higher than that of the corresponding crystals. The related excess of the low-energy vibrational states, the so-called 'boson' peak, was similarly considered to be an anomaly distinguishing glasses from crystals and related to their disordered state. Recent results [1] reveal that (i) the difference in the discussed properties occurs not because the glass is structurally disordered, but because it usually has lower density than that of the corresponding crystal, (ii) the heat capacity of glasses and crystals with same densities is quite similar, and (iii) the boson peak is the glassy counterpart of the van Hove singularity of the corresponding crystal.

We analyze the generality of the new results and discuss the compatibility of the suggested interpretation of the boson peak with available experimental data. Analyzing the relation of the new results to various theoretical models, we discuss a possible experimental approach to explore further the nature of the low-frequency vibrational excitations in glasses [2].

Corresponding Author: jan.krawczyk@ifj.edu.pl

The inelastic neutron scattering spectra were measured for two liquid crystal chiral glass-formers: (S)-4-(2-methylbutyl)-4’-cyanobiphenyl (5*CB) and (S)-4-(1-methylheptyloxy)-4’-cyano-biphenyl (8*OCB) in the temperature range from 4 to 30 K. The experiments were performed for phase I, glass of phase II and glass of cholesteric phase for 5*CB and phase II, glass of phase I and glass of isotropic liquid for 8*OCB.

Boson peak was observed for phase I and glass of phase II for 5*CB and for glass of isotropic liquid for 8*OCB (Fig. 1). For other experimental runs the boson peak was not observed or was of much less intensity. For all runs the broadening of the elastic peak, characteristic for conformational jumps or reorientation of molecular groups, was observed. The estimated correlation time of these motions was of the order of picoseconds. The tunnel splitting suggested for temperatures lower than 1 K by relaxation calorimetry experiment was not observed.
Immense elastic softening and the responsible molecular mechanisms near the demixing phase transition of thermo-responsive polymer solutions

PHILIPP, Martine 1; KYRIAKOS, Konstantinos 1; MÜLLER, Ulrich 3; LOHSTROH, Wiebke 1; PETRY, Winfried 1; PAPADAKIS, Christine 1; KRÜGER, Jan 2; MÜLLER-BUSCHBAUM, Peter 1

1 Technische Universität München, Munich, Germany; 2 Université du Luxembourg, Luxembourg, Luxembourg; 3 Universität des Saarlandes, Saarbrücken, Germany

Corresponding Author: martine.philipp@tum.de

Functional materials based on stimuli-responsive polymers are of great interest in view of their current use, and foreseen future implementation, in many everyday life applications. Frequent applications are sensors, drug delivery systems, soft robotics and responsive surfaces. The environmental responsiveness of such hydrogels, thin films or micellar solutions bases on a structural instability, which occurs at a demixing transition with a lower critical solution temperature (LCST). Even though numerous theoretical and experimental studies have been carried out, central problems regarding the phase separation mechanisms remain unsolved. Using aqueous solutions of the model thermo-responsive polymer poly(N-isopropyl acrylamide) (PNIPAM), we identify the volume expansion coefficient and the isothermal compressibility as order parameter susceptibilities of the demixing transition [1-3]. An intriguing finding based on Brillouin spectroscopy is that immense strain-softening, and hence a third order elastic constant, governs the phase separation, instead of the linear elastic properties [2]. In order to better assess the relationship with the underlying molecular mechanisms, we also focus on the molecular origins of the demixing transition [1, 4]. Important variations in hydrophobic and H-bond interactions occur within the phase-separating polymer solutions. Our studies based on quasi-elastic neutron scattering show how the local diffusion behavior of the hydration water varies during the partial dehydration of the PNIPAM chains in the course of the demixing transition [4]. Novel insights into the impact of the molecular processes on the macroscopic order parameter susceptibilities of the phase separation of stimuli-responsive polymer systems are finally given.

Creating, imaging, and transforming the topological charge in a superconductor, a superfluid, a system of cold atoms, or a soft ferromagnet is a difficult—if not impossible—task, because of the shortness of the length-scales and lack of control. The length scale and softness of defects in liquid crystals allow for the easy observation of charges, but it is difficult to control charge creation. Recently, we demonstrated [1,2] full control over the creation, manipulation and analysis of topological charges that are pinned to a microfibre in a nematic liquid crystal. Oppositely charged pairs are created via the Kibble-Zurek mechanism by applying a laser-induced local temperature quench in the presence of symmetry-breaking boundaries. The pairs are long-lived, oppositely charged rings or points that either attract and annihilate, or form a long-lived, charge-neutral loop made of two segments with a fractional topological charge. This indicates the sensitivity of the Kibble-Zurek mechanism and the coarsening dynamics of entangled defects at late times to the connectedness of space and symmetry-breaking boundary conditions which might have implications also on the cosmological level. Furthermore, we show that any even number of topological charges could be deliberately created on topologically simple objects, which opens new routes to the design and assembly of topologically complex colloidal structures.

Multiferroics and ferroelectrics

High resolution polarized Raman scattering study of multiferroic MnWO₄

ZIEGLER, Fabian ¹; GIBHARDT, Holger ¹; LEIST, Jeannis ¹; ECKOLD, Götz ¹; BECKER, Petra ²; BOHATÝ, Ladislav ²
¹ Georg-August-Universität Göttingen, Göttingen, Germany; ² Universität zu Köln, Cologne, Germany

Corresponding Author: fziegle@gwdg.de

Multiferroic materials with magnetic and electric ordering within a single phase gained attention during the last years due to their potential for industrial applications. Materials with a cycloidal spin arrangement are of particular interest because the electrical polarization is directly caused by the complex magnetic order. Hence, both ordering phenomena are tightly coupled in this category of compounds. One example is MnWO₄, which passes successively three antiferromagnetic phase transitions on cooling. The phase AF2 between 12.5 K and 7 K exhibits a cycloidal spin arrangement with an incommensurate magnetic propagation vector. This ordering induces a spontaneous polarization by the inverse Dzyaloshinski-Moriya-interaction. As a consequence, the interaction between spin and polarization could possibly lead to a change in the spectrum of lattice vibrations. Due to the tiny polarization, it was believed up to now that this effect was too small to be observed experimentally. Using high resolution polarized Raman scattering, however, we were able to detect clear signatures of this magnetoelectric interaction. The Raman spectra were taken from a MnWO₄ single crystal in the temperature range from 100 K to 6 K covering the three magnetic phase transitions. A careful analysis of the experimental data allowed the precise determination of both, the wave numbers and intrinsic linewidths. Most of the 18 Raman-active phonons show a significant shift in wave number below the magnetic ordering temperature that cannot be explained merely on the basis of lattice dynamics, but should be attributed to spin-phonon-interaction. The most striking effect is observed for the Ag mode with the highest frequency (about 884 cm⁻¹), which corresponds to an oxygen stretching vibration and exhibits a pronounced softening on cooling.
Néel-type Skyrmion Lattice in a Polar Magnetic Semiconductor

KÉZSMÁRKI, István 1; BORDÁCS, Sándor 1; WHITE, Jonathan 2; MILDE, Peter 3; MOCHIZUKI, Masahito 4; TSURKAN, Vladimir 5; LOIDL, Alois 6
1 Budapest University of Technology and Economics, Budapest, Hungary; 2 Paul Scherrer Institut (PSI), Villigen, Switzerland; 3 Technische Universität Dresden, Dresden, Germany; 4 Aoyama Gakuin University, Sagamihara-cho, Japan; 5 University of Augsburg, Augsburg, Germany

Corresponding Author: kezsmark@dept.phy.bme.hu

Following the early prediction of the skyrmion lattice (SkL)—a periodic array of spin vortices—by Bogdanov and coworkers [1], it has been observed recently in various magnetic crystals mostly with chiral structure [2]. Although non-chiral but polar crystals with Cnv symmetry were identified as ideal SkL hosts in pioneering theoretical studies, this archetype of SkL has remained experimentally unexplored. Here, we report the discovery of a SkL in the polar magnetic semiconductor GaV₄S₈ with rhombohedral (C₃ᵥ) symmetry and easy axis anisotropy [3]. The SkL exists over an unusually broad temperature range compared with other bulk crystals and the orientation of the vortices is not controlled by the external magnetic field but instead confined to the magnetic easy axis. Supporting theory attributes these unique features to a new Néel-type of SkL describable as a superposition of spin cycloids in contrast to the Bloch-type SkL in chiral magnets described in terms of spin helices. We found that the strong orientational confinement of the vortices ensures the robustness of two distinct skyrmionic states with a core magnetization pointing either up or down the easy axis. This may facilitate a unique magnetic control of the SkL by magnetic fields applied perpendicular to the vortex cores in contrast to cubic helimagnets where vortex cores instantaneously co-align with the magnetic field. In addition, the polar crystal structure of GaV₄S₈ may be exploited for a non-dissipative electric field control of the SkL.


Fig. 1: Left: Magnetic phase diagram of GaV₄S₈ including the cycloidal, SkL and ferromagnetic states. Middle: Atomic force microscopy image about the magnetic pattern in the SkL phase. Right: Small angle neutron scattering image representative of the cycloidal phase taken at zero magnetic field.
The lacunar spinel GaV$_4$S$_8$ undergoes orbital ordering at 44 K and reveals a complex magnetic phase diagram below 13 K, including a ferromagnetic, cycloidal and Néel-type skyrmion lattice phase.[1] Skyrmions are topologically protected nano-scale spin vortices with fascinating physical properties and high potential for future data storage. Based on magnetic susceptibility, heat capacity and pyrocurrent measurements, all as function of temperature and magnetic field, we construct a detailed phase diagram and in addition, we provide a thorough study of the polar properties of GaV$_4$S$_8$, revealing that its orbitally ordered phase is ferroelectric with sizable polarization of ~ 1 μC/cm$^2$. Moreover, spin-driven excess polarizations emerge in all magnetic phases; hence, GaV$_4$S$_8$ hosts three different multiferroic phases including the skyrmion lattice formed by ferroelectric spin vortices.[2] By taking into account the crystal symmetry and spin patterns of the magnetoically ordered phases, exchange striction is identified as the main microscopic mechanism behind the spin-driven ferroelectric polarization in each multiferroic phase. The polar crystal structure of GaV$_4$S$_8$ is unique among the known skyrmion-lattice host materials and the ferroelectric SkL phase may be exploited for non-dissipative electric-field control of skyrmions.

In the second part of this talk we present detailed results using THz and coplanar waveguide (CPW) absorption spectroscopy. We find an intriguing relaxation dynamics in the THz range indicating the divergence of relaxation times coupled to the orbital dynamics and establishing an orbitally driven ferroelectric phase below the Jahn-Teller transition. In addition, using CPW absorption spectroscopy we study magnetic excitations of the skyrmion, the helical and the collinear spin phases.[3]

Broadband THz spectroscopy is a very useful tool to study complex magnetic/electric order in condensed matter i.e. in multiferroic compounds since both magnetic (magnons) and electric (optical phonons) excitations lie in this energy range. When cross coupling between magnetic and electric order occurs, new kind of excitations may emerge: these are called electro-magnons. Coupling two complementary experimental techniques, THz/FIR spectroscopy on synchrotron source and inelastic neutron scattering, we have focused on two members of the multiferroics hexagonal manganites RMnO$_3$, with R=Er and Ho. These compounds order electrically below 800 K and magnetically around 80 K with a 120° frustrated arrangement of the Mn$^{3+}$ ions. We have fully characterized the low energy spectra (magnon, phonon, crystal field transitions) of these compounds and their excitation rules as regards the electric and magnetic fields of the THz wave. In ErMnO$_3$, we have observed the complete loss of the magnetic character of a magnon transmuted into an electroactive excitation [Chaix, et al. Phys. Rev. Lett. 112, 137201 (2014)]. We attribute this magnetoelectric dynamical process to the hybridization between a crystal field level transition of the Er magnetic rare earth and a Mn magnon. In HoMnO$_3$, spectacular modifications of the Mn spin waves and Ho crystal field level transitions are observed at a temperature of 40 K when a spin reorientation of the Mn$^{3+}$ magnetic moments occurs, together with the ordering of some Ho ions. At lower temperature, the spin waves dispersion perpendicular to the Mn triangular planes vanish, the Mn ordered structure being maintained in the molecular field of the rare earth ions. Both studies highlight the crucial role of the strong coupling between Mn and rare earth ions in the dynamical properties of these hexagonal manganites.
Multiferroics, where spontaneous long-range magnetic and polar orderings coexist, represent an attractive class of compounds combining rich physics with potential for multifunctional applications. TbMnO$_3$ and DyMnO$_3$ are multiferroics compounds exhibiting magnetic ordering of Mn$^{3+}$ ions, with a sinusoidal modulated collinear structure below $T_N$ = 41 K and 39 K, and a cycloidal one below $T_{\text{lock}}$ = 27 K and 18 K, respectively, which is accompanied by the emergence of spontaneous electric polarization [1,2], accordingly to the Dzyaloshinskii-Moriya model [3]. Usually, the magnetoelectric coupling has rather small magnitude. However, larger magnetoelectric effect can be found in frustrated magnetic materials. In rare-earth perovskite manganites, the magnetic frustration can be induced by modifications of exchange interactions among nearest and next-nearest neighbors of Mn$^{3+}$. To tune the balance between these ferro and antiferromagnetic interactions, we have studied the effect of Mn$^{3+}$ substitution by Fe$^{3+}$ on selected physical properties of TbMn$_{1-x}$Fe$_x$O$_3$, with $x = 0$ to 0.05, and DyMn$_{1-y}$Fe$_y$O$_3$, with $y = 0$ to 0.03, since Fe$^{3+}$ has the same ionic radius as Mn$^{3+}$ but it is not Jahn-Teller active. This substitution induces small structural distortions and changes the magnetic interactions, already at $x = 0.05$ and $y = 0.03$ the ferroelectricity is lost. Interestingly though, within this range, as $x/y$ increases there is a strong increase of the magnetoelectric effect. The polarization becomes so sensible to the magnetic field, that for the highest $x/y$, it can be almost suppressed. The magnetoelectric ($x/y, T$) phase diagrams are proposed.

Corresponding Author: elsa.lhotel@neel.cnrs.fr

Geometrically frustrated magnetic systems provide a large variety of unusual magnetic ground states. Among these, the pyrochlore oxide compounds (formula $A_2B_2O_7$, where $A$ is a magnetic rare-earth, and $B$ a transition metal) have focused much attention, because their lattice, made of corner-sharing tetrahedra, is a source of strong magnetic frustration. It results in the stabilization of exotic magnetic ground states, such as classical or quantum spin-ices, spin-liquids or unconventional magnetic orders combined with spin fluctuations. I will present a review of magnetization and ac susceptibility studies on these compounds which evidence the existence of slow dynamics at very low temperature. These dynamics coexist with fast fluctuations and / or magnetic ordering. They can be the signature of emergent excitations, such as magnetic monopoles in classical spin-ices ($A=Ho, Dy$) but in other systems ($A=Tb, Er, Nd...$), their origin remains an open issue. They could be due to loop dynamics, domain-wall dynamics, as well as induced by the presence of structural defects.

Figure 1: Relaxation of the magnetization induced by the magnetic monopoles hopping at very low temperature in the spin-ice compound Dy$_2$Ti$_2$O$_7$. The relaxation is enhanced below 500 mK by an excess of magnetic monopoles density, created through the Avalanche Quench process (AQ - red), compared to the case of conventional cooling (CC - blue). (from C. Paulsen et al., Nature Phys. 10, 135 (2014))
One of the biggest dreams in solid-state physics is getting quantitative access to the dynamical properties of tiny-tiny systems in real time and real space. Any technique that averages over an ensemble behavior thus inherently cannot be used and is out of scope here. Equally, indirect k-space methods will fail at these small length scales as well, due to the same limitations.

In order to fulfill the above requests, we recently developed scanning-probe-methods (SPM) towards both a superb spatial and temporal resolution. The high spatial resolution is inherently known in SPM from tons of splendid works performed on metallic, semiconducting, insulating, organic and biological nanomaterials, reporting a topographic resolution down to the single atomic and molecular level. What is novel, though, is that these SPM methods can be easily tuned towards an unprecedented time resolution down to pico-seconds. We will introduce into these novel techniques with two examples of solid-state measurements. The first system addresses ultrafast electronic transport properties as exemplified on a thin film organic field-effect transistor (OFET). To monitor the charge recombination in-situ we modified a standard non-contact scanning force microscope (nc-SFM) operated in the Kelvin force probe mode (KPFM) to measure surface potentials, into a time-resolved KPFM (tr-KPFM) technique [1]. tr-KPFM is able not only to delineate and track the charge wave fronts of injected electrons in real time, but equally proves, why today’s OFET devices fail to achieve faster switching speeds, simply due to Schottky barrier issues.

The second example will be discussed by quantifying the excited state lifetime of electrons in an optically pumped SiGe semiconductor device [2]. Here, a similar side-band demodulation scheme as for tr-KPFM is implemented into scattering scanning near-field optical microscopy (tr-s-SNOM). We find the charge carrier lifetimes to drastically depend on their ground state population density, as monitored by varying the Si-to-Ge concentration.

Electrons and spins

Domain wall dynamics, local diffusion, and phonons in a lead-free relaxor ferroelectric

PFORR, Florian 1; MAJOR, Marton 1; STUHR, Uwe 2; ROESSLI, Bertrand 2; IVANOV, Alexandre 3; DONNER, Wolfgang 1
1 Technische Universität Darmstadt, Darmstadt Germany; 2 Paul Scherrer Institut (PSI), Villigen, Switzerland
3 Institut Laue-Langevin (ILL), Grenoble, France

Corresponding Author: pforr@st.tu-darmstadt.de

Ferroelectric materials are used in many applications, e.g. as ultrasonic transducers. The most commonly used ferroelectrics like Pb\textsubscript{x}Zr\textsubscript{1-x}TiO\textsubscript{3} contain lead, which makes them potential hazards for human health and our environment. Consequently, lead-free ferroelectrics are currently being developed with the aim of replacing the lead-containing materials in the medium term. However, the microscopic mechanisms which determine the ferroelectric properties have to be identified before the properties can be optimized for specific applications.

The ferroelectric parameters of solid solutions near the morphotropic phase boundary of Bi\textsubscript{1/2}Na\textsubscript{1/2}TiO\textsubscript{3}-BaTiO\textsubscript{3} around x = 0.06 were cited as d\textsubscript{33} = 125 pC/N and \varepsilon\textsubscript{33}T / \varepsilon\textsubscript{0} = 580. These values are comparable to those of commonly used lead-containing ferroelectrics. The diffuse x-ray scattering experiments performed by our group revealed features related to the local octahedral tilting order and stacking faults between different tilt domains. These features react strongly to the application of an external electric field and their temperature dependence is clearly correlated with the dielectric permittivity. Potential phonon anomalies may also help to identify the mechanisms leading to the good ferroelectric properties.

We investigated the temperature dependence of the structural dynamics of a single crystal with x = 0.04 using inelastic and quasielastic neutron scattering. Most phonon branches are not well defined, but hints of possible anomalies are visible. The quasielastic scattering (QENS) was measured at different positions in reciprocal space, focusing on the field-dependent diffuse scattering. We observed a very strong temperature and Q dependence. This indicates that different mechanisms like enhanced domain wall mobility and local cation hopping strongly influence the dielectric properties in different temperature ranges.
Metal borohydrides: from hydrogen storage to electrochemistry

ŁODZIANA, Zbigniew

1 Institute of Nuclear Physics, Polish Academy of Science, Cracow, Poland

Corresponding Author: zbigniew.lodziana@ifj.edu.pl

Metal borohydrides (M-BH₄) have focused research attention due to large hydrogen content. Extensive basic research efforts were directed toward understanding their dynamical and thermodynamic properties. Unfortunately, till now none of such compounds meets practical requirements for reversible hydrogen storage. The unexpected side effect of such research was discovery of the high ion mobility in pure or ion substituted LiBH₄. Even more surprising was the discovery of high sodium mobility in decomposition products of NaBH₄ containing large B₁₂H₁₂ anions. All these effects are related to the dynamical properties of systems with small non-spherical ions that will be presented from theoretical perspective during the talk.
We report on the atomic dynamics in a glass-forming Au$_{81}$Si$_{19}$ liquid using quasielastic neutron scattering. At low q-values and high temperatures the self-diffusion of gold is well approximated in the hydrodynamic approach with a simple exponential describing the final decay of the self-correlation function. With increasing q, we observe a systematic stretching of the correlation functions, indicating the existence of dynamical heterogeneities with decreasing observation length scale even at high temperatures in the equilibrium liquid. A dynamic crossover from the hydrodynamic regime to that of heterogeneous dynamics was observed to occur close to the liquidus temperature. There, a pronounced stretching of the correlation functions over the entire investigated q-range is apparent, which suggests the onset of structural arrest. Despite the glass-forming nature of this system, the self-diffusivity obeys an Arrhenius law characteristic of simple liquids, without any apparent signature of a dynamic singularity in the investigated temperature range. This is most likely due to the very fragile nature of this system, in which the microscopic dynamics exhibits characteristics of both simple and glass-forming liquids.
Shining light on atomic hopping processes - diffusion mechanisms in B2 alloys

Corresponding Author: markus.stana@univie.ac.at

While diffusion is well understood for pure metals and for solid solutions, diffusion mechanisms in ordered intermetallic alloys are still under debate. Even for the simple case of B2 alloys, very little is known. As nearest-neighbour jumps would destroy the long-range order, effective jumps to further neighbouring shells have to be considered. Such jumps can either take place directly, where the atom has to overcome a large energy barrier, or as a fast sequence of nearest-neighbour jumps. The later can be described by different jump mechanisms among which the six-jump mechanism and the triple defect mechanism are most famous.

We use coherent X-rays to find wave-vector dependent relaxation times in different systems. By extending X-ray Photon Correlation Spectroscopy, which is the X-ray analogue of Dynamic Light Scattering, to wide angles [1], it is possible to gain information about diffusion in different materials [2,3,4]. In binary intermetallic alloys it is possible to determine the length and rate of effective atomic jumps. The ratios of jump-rates are compared to jump models.

This talk will give a brief introduction to atomic-scale X-ray Photon Correlation Spectroscopy and compare results about diffusion constants, activation energies and jump models as well as the influence of short-range order in the B2 systems Fe-Al and Ag-Mg.

The study of friction and diffusion processes on molecular length scales requires experimental methods that deliver sub-nanometer spatial resolution at nanosecond time resolution. After decades of research in friction the range of available spectrometers with these characteristics is still too limited. Although, neutron scattering is not a widely used for surfaces, neutron spectroscopy is able to cover the space and time domains that are of interest here. In addition, a wide choice of high surface density materials are available now that can serve as substrates for diffusion studies. These materials have the added benefit, that they are widely applied in energy storage, sensing and filtering. Hence, research on these materials has strong potential technical impact. In this presentation, we will show recent progress in friction research using neutron spectroscopy and diffraction. Our research started with rather small and structurally simple molecules on carbon substrates, such as the aromatic molecule benzene adsorbed on the basal plane surface of graphite(0001) [1,2]. For benzene-graphite(0001) at sub-monolayer coverage, we now established the inter-molecular energy dissipation and the surface friction [2] using a range of neutron time-of-flight spectrometers, neutron spin-echo as well as neutron diffraction. The results led us to a surprisingly simple model: the inter-molecular friction can be quantitatively explained by a model of colliding cogwheels (or rough hard disks) that we had developed on the basis of the long established rough hard sphere model for molecular gases (the equivalent 3D model). The new model explains the collisional friction or viscosity based on universal constants only and makes almost no assumptions about the system.

J.W. Gibbs founded the field of materials science, basing it on the concept of free energy, $G = E - TS + PV$. For the past century, free energies of materials have been tabulated from measurements of heat capacities, which do not identify the physical sources of enthalpy and entropy. For the past 30 years, it has often been possible to calculate $E$ and $PV$, but the entropy $S$ has remained more difficult.

Most of the entropy $S(T)$ comes from atomic vibrations, i.e., phonons. The phonon entropy is big, small fractional differences are important, and the harmonic approximation is not sufficiently accurate to be useful for materials thermodynamics at elevated temperatures. Ab initio molecular dynamics (AIMD) has proved a versatile approach for calculating the phonon entropy at elevated temperatures, including the parts from phonon-phonon and electron-phonon interactions. The results have enough accuracy so that a calculated $S(T)$ can compete with $S(T)$ from calorimetry. Almost in parallel, inelastic scattering methods have become capable of determining the phonon entropy to similar accuracy. AIMD simulations can also provide Van Hove space-time correlation functions, allowing comparisons to results from inelastic scattering experiments by at the level of individual phonon modes (rather than comparing an integral quantity like $S$). The entropy of fcc Al metal has been determined by calorimetry, AIMD, many-body perturbation theory, and inelastic neutron scattering. Although fcc Al is modestly anharmonic, these four different results for entropy agree well. Other cases of cubic Ag$_2$O and rutile TiO$_2$ show enormous phonon-phonon anharmonicity, but the AIMD results are still consistent with experimental phonon measurements. With thermal expansion, several modes in rutile TiO$_2$ are known to become unstable in the quasiharmonic approximation. From AIMD simulations it was found that the bottom of the Ti-O interatomic potential flattens with temperature, giving a quartic character that stabilizes the rutile structure.

Understanding $S(T)$ is essential for the practical design and use of materials at finite temperatures. Inelastic scattering is a natural partner to ab initio simulations, offering important validations. Likewise, the simulations give deeper insights into the experimental results. The time is ripe for better connections between computational materials science and inelastic scattering research.
The interactions of spin, lattice and electronic degrees of freedom in materials are at the origin of complex phase diagrams resulting in new emergent phenomena and technical applications. The coupling between lattice and electronic degrees of freedom is well understood, and the interaction between spin and electronic excitations has been investigated intensely, e.g., in the research on high-temperature superconductivity. However, only little is known about the dynamic interactions between spin and lattice excitations, apart from the well-established magneto-elastic coupling. Noncentrosymmetric FeSi is known to undergo a transition from insulating to metallic behavior with increasing temperature, and exhibits strongly temperature dependent phonon energies. Here we show by detailed inelastic neutron scattering measurements that the phonon renormalization in FeSi is in fact linked to its unconventional magnetic properties. In combination with ab-initio calculations, we demonstrate that two different mechanisms cause the unusual behavior: Electronic states mediating conventional electron-phonon coupling are only activated in the presence of strong magnetic fluctuations. Secondly, phonons are damped via a dynamic coupling to the temperature-induced magnetic moment with the highest impact on phonons having strongly varying Fe-Fe distances. Our findings highlight FeSi as one of the rare materials with direct spin-phonon coupling and a prime example for multiple interaction paths.
Corresponding Author: neugebauer@mpie.de

A key requirement in developing systematic approaches to explore and predict properties of materials not yet synthesized is the availability of accurate computational tools determining energies not only at $T = 0$ K but also under realistic finite temperature conditions. A critical step towards this goal is the ability to accurately describe all relevant excitation mechanisms such as phonons, magnons, excited electrons. For many scientifically and technologically important functional as well as structural materials the various excitation mechanisms are not adiabatically decoupled but non-adiabatic couplings e.g. between magnons and phonons or between electrons and photons (electron-phonon interaction) become critical and need to be included for an accurate description of their thermodynamic properties.

In the talk we will show how novel sampling strategies in the atomic configuration space together with techniques to address the spin-degrees of freedom including spin-quantization in magnetic materials allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. While in the past the focus has been mainly on the quasiharmonic contributions (which are computationally most easily to obtain) recent advances provide now for the first time the opportunity to systematically include anharmonic and magnetic contributions all the way up to the melting temperature. The flexibility and the predictive power of these approaches to describe these complex excitation and coupling mechanisms will be discussed for selected materials such as ultra-high strength steels, magnetic shape memory alloys or light-weight alloys.
Lead zirconate (PZO) has been recently a subject of intensive studies with its antiferroelectric (AFE) phase transition (PT) being in a spotlight. Since there is no direct link between the paraelectric cubic phase and the low temperature orthorhombic one, the process leading to the emergence of AFE order is not obvious. Results of X-ray inelastic as well as Brillouin scattering experiments has directed Tagantsev et al. to propose a flexoelectric coupling to be the main physical mechanism behind the AFE PT [1]. On the other hand, Hlinka et al. on the basis of infra-red, Raman and THz spectroscopy as well as group theory considerations proposed an alternative picture of the PT mechanism where soft ferroelectric branch is coupled by a trilinear term to two oxygen octahedra tilt modes [2].

We present a shell model molecular dynamics study of PZO. This recently developed model has already been used for explanation of X-ray [3] as well as neutron diffuse scattering data [4]. Very good agreement between modeled and experimental intensities (coming mostly from phonons) assures that the model correctly describes dynamics of the system. The atomistic simulation allows us to study theoretically phonons at finite temperatures (for the first time for PZO). To shed the light on the emergence of the AFE order, we concentrate on the cubic phase and show how the lattice dynamics changes towards the phase transition.

This work is supported by the Czech Science Foundation (project no. 13-15110S). The computational part of this research was undertaken on the NCI National Facility in Canberra, Australia.

Theoretical and experimental methods

Polarized Raman Spectra of Perovskite Relaxor Ferroelectrics

HLINKA, Jiří

1 Academy of Sciences of the Czech Republic (AS CR), Prague, Czech Republic

Corresponding Author: hlinka@fzu.cz

Pseudo-binary solid solutions of perovskites ferroelectrics are often showing either a ferroelectric transitions with a glassy dynamics or enhanced piezoelectric properties. Because of the demonstrated application potential of \((1-x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3-x\text{PbTiO}_3\) and related materials, considerable research efforts are still payed to the understanding these phenomena.

The IR spectroscopy of such lead-based perovskites is relatively well understood[1], but the assignment of Raman spectra remains a rather difficult task. The Raman activity seems to originate from both the occupational ordering [2] and the ionic off-centering [3]. The weight of these effects is varying from one material to another. Moreover, the inherent disorder seems to lift the strict Raman selection rules. Interestingly, the polarized Hyper-Raman scattering spectra obey the standard polarization selection rules rather well [4,5] Nevertheless, Raman scattering in relaxors shows a measurable polarization dependence and it has been argued that specific features of polarised Raman scattering can be even employed for example to probe relaxor to ferroelectric crossover [6] or to distinguish between distinct ferroelectric phases coexisting in materials with composition close to the so-called MPB boundaries [7].

Here we shall present our recent polarized Raman scattering studies of relaxors. In the spirit of Dyproso symposium, we shall go through the basic concepts, challenges and unpublished results.

Corresponding Author: alain.sacuto@univ-paris-diderot.fr

The pseudogap phase in cuprates remains hitherto a mysterious state of matter out of which the high-temperature superconductivity emerges. Discovered more than twenty five years ago [1], its indentification is still challenging although extensively studies have been carried out to elucidate its true nature [2,3]. In addition recent investigations in the underdoped side of the cuprate phase diagram have shown inside the pseudogap phase the existence of charge density wave order [4-6] which could be at the origin of the Fermi surface reconstruction in electron and hole pockets detected at high magnetic field by quantum oscillations [7,8] and transport measurements [9]. Instead of clarifying our understanding of the cuprate phase diagram, these recent investigations have revealed its unexpected complexity. In this context our purpose is to reveal by electronic Raman scattering, the signature of the normal state pseudogap and track its doping evolution through the cuprate phase diagram. We will demonstrate there exists a direct connection between Raman and transport measurements on the pseudogap. Although intensively studied in the underdoped regime, relatively less is known about the normal state pseudogap on the overdoped side, where it weakens and eventually disappears at a critical doping \( p_c \). Here, combining Raman spectroscopy on Bi-2212 over a large range of finely tuned doping with theoretical calculations, we determine \( p_c = 0.22 \) and we show that it coincides with a Lifshitz transition where the underlying hole-like active Fermi surface becomes electron-like [10]. Interestingly, the superconducting critical temperature \( T_c \) is unaffected by this transition. This demonstrates that the microscopic origins of the normal state pseudogap and the superconductivity are distinct. Only the former is tied to the change in the Fermi surface topology.

Excitations of strongly correlated electron systems

New insights on the cuprates phase diagram from x-ray scattering

LE TACON, Matthieu

1 Max Planck Institute for Solid State Research, Stuttgart, Germany

Corresponding Author: m.letacon@fkf.mpg.de

I will present an overview of the results obtained from various x-ray scattering experiments on high temperature superconducting cuprates in the last couple of years.

I will first focus on Cu L-edge resonant scattering experiments that led us to uncover charge density wave (CDW) correlations competing with superconductivity in the YBCO family, for which a complete temperature and doping dependent phase diagram has been worked out.

These investigations have been extended to other families of cuprates (Bi2201, Bi2212 and Hg1201) demonstrating the ubiquity and the universality of the phenomenon.

Further information was gained from high resolution inelastic x-ray scattering. The observation of a quasi-elastic ‘central peak’ unraveled the static nature of the CDW correlations, attributed to the pining of CDW nanodomains on defects. Low energy phonons exhibit anomalously large superconductivity induced renormalizations close to the CDW ordering wave vector, providing new insights regarding the long-standing debate of the role of the electron-phonon interaction, a major factor influencing the competition between collective instabilities in correlated-electron materials.

Finally I will discuss new results obtained in a heterostructure comprising YBCO and metallic ferromagnet La$_{2/3}$Ca$_{1/3}$MnO$_{3}$, where a stabilization of the CDW phase is concluded and discussed within the scope of tuning the equilibrium conditions of metastable phases via heterostructuring.
Excitations of strongly correlated electron systems

Magnetic resonant excitations in S-doped iron-chalcogenide superconductors

PARK, Jitae

1 Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany

Corresponding Author: jitae.park@frm2.tum.de

A sharp magnetic collective mode appearing inside the superconducting energy gap in the spin excitation spectrum is a smoking-gun evidence for phase-reversed electron-pairing symmetry in unconventional superconductors. Such mode has been observed by inelastic neutron scattering in many of iron-based superconductors, in which the phase-reversed $s$-wave pairing symmetry had been proposed. Yet, it is still under an active debate about the exact pairing symmetry of recently discovered 122-type iron-chalcogenide despite the presence of the spin resonant mode mostly due to the absence of hole Fermi surface at the Brillouin zone center. Here, we present a systematic study of inelastic neutron scattering on the sulfur-doped iron-chalcogenide $K_xFe_{2-y}(Se_{1-z}S_z)_2$ [$z=0,0.25,0.4,0.5$] to clarify how S-doping affects to the spin fluctuations and the magnetic resonant excitations. Further, we discuss the physical implication of our inelastic neutron scattering data based on the tight relationship between the magnetic resonant mode and superconducting order parameter symmetry.
Experimental and theoretical studies of the lattice dynamics in superconducting BaNi$_2$(As$_{1-x}$P$_x$)$_2$

FORREST, Thomas $^1$; WEHINGER, Björn $^2$; BOSAK, Alexei $^1$; ROTUNDU, Costel $^3$

$^1$European Synchrotron Radiation Facility (ESRF), Grenoble, France; $^2$University of Geneva, Geneva, Switzerland; $^3$Stanford University, Stanford, USA

Corresponding Author: thomas.forrest@esrf.fr

We present a combination of Thermal Diffuse Scattering (TDS) and Inelastic X-ray Scattering (IXS) measurements, and Density Functional Perturbation Theory (DFPT) calculations of the lattice dynamics in superconducting BaNi$_2$(As$_{1-x}$P$_x$)$_2$. At $T_s$=130 K, BaNi$_2$As$_2$ undergoes a structural phase transition from a tetragonal to a triclinic crystal structure. In addition, superconductivity emerges at $T_c$= 0.7 K. Substitution of the arsenic with phosphorus leads to a suppression of $T_s$. Finally, at a substitution level of 7%, the structural phase transition is completely suppressed and the $T_c$ jumps from 0.7 to 3.3 K. It is believed that the nature of the superconductivity displayed by this material is of the conventional BCS type. Furthermore, specific heat measurements suggest that a “Giant” phonon softening is responsible for the jump in $T_c$. In order determine if such a large phonon softening does occur in BaNi$_2$(As$_{1-x}$P$_x$)$_2$, we have undertaken a combined experimental and theoretical study of the lattice dynamics of this material. TDS measurements on BaNi$_2$As$_2$ have identified locations of significant diffuse scattering. Upon cooling, the scattering from these diffuse regions becomes stronger, collapsing into true Bragg structural reflections below $T_s$. The IXS measurements and DFPT calculations identify this to be the location of a significant softening of at least one phonon mode. Out results demonstrate that these phonons are strongly coupled to the structural phase transition, and therefore it is a strong candidate for being responsible for the jump in $T_c$. In order to ascertain if this is correct, we have extended our TDS and IXS measurements to phosphorus doped BaNi$_2$As$_2$. Results from these latest set of measurements will be presented. In addition, our results will be compared to the lattice dynamics to the iron pnictide unconventional superconductors.
Recently, it has become widely accepted that charge ordering is a universal property of hole doped high-temperature cuprate superconductors [1-6]. This talk gives an overview of the current experimental effort to reveal the nature of the charge density wave order. Special focus will be given to x-ray diffraction experiments. Implications for the Fermi surface reconstruction and superconductivity will be discussed along with possible connections to pseudogap physics.

Layered triangular antiferromagnet selenide AgCrSe$_2$ (SG: R3m) has been investigated by means of elastic and inelastic neutron scattering, combined with electrical transport, Seebeck coefficient, magnetisation and heat conductivity ($\kappa$) measurements, in the range 5 to 300 K. Below $T_N = 55$ K [1], long-range magnetic ordering is identified, characterized by long-wavelength incommensurate antiferromagnetic cycloids running along [110], and rotating within the ab plane ($k = e e 3/2$). No structural transition is observed down to 1.5 K, in contrast with structural parent AgCrS$_2$ [2]. Spin wave modelling of the inelastic scattering spectrum in the magnetically ordered phase leads to ferromagnetic and antiferromagnetic exchange interactions between nearest and next-nearest neighbours, respectively, with a weak antiferromagnetic interplane exchange. The most remarkable features of the excitation spectra are a 3 meV phonon with an anomalous temperature behaviour above 80 K, and the persistence of a magnetic signal up to 150 K ($\sim 3 T_N$). The presence of this low energy phonon is in agreement with the extremely low thermal conductivity of AgCrSe$_2$, which is attributed to phonon scattering by Ag$^+$ rattling; on the other hand, the absence of any magnetic field effect (up to 9T) on $\kappa$ suggests the absence of any additional contribution to the heat conduction from magnons [3].

Layered triangular antiferromagnet selenide AgCrSe$_2$ (SG: R3m) has been investigated by means of elastic and inelastic neutron scattering, combined with electrical transport, Seebeck coefficient, magnetisation and heat conductivity (kappa) measurements, in the range 5 to 300 K. Below $T_N = 55$ K [1], long-range magnetic ordering is identified, characterized by long-wavelength incommensurate antiferromagnetic cycloids running along [110], and rotating within the ab plane ($k = e e 3/2$). No structural transition is observed down to 1.5 K, in contrast with structural parent AgCrS$_2$ [2]. Spin wave modelling of the inelastic scattering spectrum in the magnetically ordered phase leads to ferromagnetic and antiferromagnetic exchange interactions between nearest and next-nearest neighbours, respectively, with a weak antiferromagnetic interplane exchange. The most remarkable features of the excitation spectra are a 3 meV phonon with an anomalous temperature behaviour above 80 K, and the persistence of a magnetic signal up to 150 K ($\sim 3 T_N$). The presence of this low energy phonon is in agreement with the extremely low thermal conductivity of AgCrSe$_2$, which is attributed to phonon scattering by Ag$^+$ rattling; on the other hand, the absence of any magnetic field effect (up to 9T) on kappa suggests the absence of any additional contribution to the heat conduction from magnons [3].

“Half-moon” excitations in the magneto-elastic spin liquid Tb$_2$Ti$_2$O$_7$

PETIT, Sylvain $^1$; ROBERT, Julien $^1$; BONVILLE, Pierre $^1$; MIREBEAU, Isabelle $^1$; DECORSE, Claudia $^1$; OLLIVIER, Jacques $^2$; MUTKA, Hannu $^3$; GUITTENY, Solène $^1$

$^1$ CEA, Centre de Saclay, Gif sur Yvette, France; $^2$ Université Paris-Sud, Paris, France; $^3$ Institut Laue-Langevin (ILL), Grenoble, France

Corresponding Author: sylvain.petit@cea.fr

Geometrical magnetic frustration is a central concept in condensed matter physics. In this field, rare earth pyrochlore magnets R$_2$Ti$_2$O$_7$ (R is a rare earth) play a prominent role, as they form model systems showing a rich variety of ground states, depending on the balance between dipolar, exchange interactions and crystal field [1]. The Terbium compound Tb$_2$Ti$_2$O$_7$ remains a cooperative paramagnet, or a “quantum spin ice”, with strongly correlated moments still fluctuating at 50 mK [2]. Recent time of flight neutron and triple-axis neutron scattering experiments have recently shed light in this puzzle, revealing a complex “magneto-elastic” ground state [3,4] characterized by a local constraint resulting in “pinch points” [5], analogous to the ice rule in spin ices, and supporting a low energy (bosonic) excitation [4]. Under applied field, a complex antiferromagnetic structure sets in, while the low energy excitations transform into a spin wave like mode whose dynamical structure factor is highly anisotropic, showing “half-moons” in reciprocal space [6]. This peculiar form indeed casts light on the underlying “ice rule” of Tb$_2$Ti$_2$O$_7$.

Phonons and magnons

Temperature dependence and linewidths of Al phonon dispersions

NEIBECKER, Pascal 1; PETRY, Winfried 1; LEITNER, Michael 1; KLAUDIA, Hradil 1; NEUGEBAUER, Jörg 2; HICKEL, Tilmann 2; GLENSK, Albert 2; GRABOWSKI, Blażej 2; NEUHAUS, Jürgen 1

1 Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany; Technische Universität München, Munich, Germany; 2 Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Corresponding Author: pascal.neibecker@frm2.tum.de

The availability of accurate phonon dispersions for all temperatures up to the melting point is essential for the prediction of thermodynamic stabilities of crystal structures. Standard ab initio approaches are based on a quasiharmonic (QH) approximation of the interaction potential, where temperature dependencies enter only via the volume expansion. We have recently developed an extension of the QH approach [1] that uses the asymmetry of the nearest-neighbor potential. The approach allows us to perform computationally efficient molecular dynamics simulations with full ab initio accuracy. The predictive power of the resulting temperature dependencies and phonon linewidths is determined in this study. We have chosen Al for this purpose, since it is isotopically pure, non-magnetic and its electronic structure is known to be adequately described by density-functional theory.

Here, we report for the first time measurements of the entire phonon dispersion of Al at temperatures of 293 K, 700 K, 800 K and 900 K, as well as at high symmetry points at additional temperatures between 15 K and 700 K. The experiments were performed at the thermal triple axis neutron spectrometer PUMA at FRM II in Garching, Germany. The presented results give access to the temperature dependent longitudinal and transversal phonon branches in the high symmetry directions including the evaluation of phonon broadening. The combination of the comprehensive theoretical and experimental data allows an evaluation of anharmonic contributions beyond Grüneisen theory to the phonon dispersion and of the temperature dependence of phonon linewidths in metals.

Corresponding Author: wilfried.schranz@univie.ac.at

Since structural changes in materials usually couple to strain, acoustic spectroscopy provides a very sensitive tool for the study of dynamic properties of solids and liquids. In principle a frequency range from 0.01 Hz up to GHz or even THz can be covered with different methods, including Dynamic Mechanical Analysis (DMA), Resonance techniques, Ultrasonics, Brillouin – and neutron scattering.

Here we present DMA measurements (0.01 – 100 Hz) for a broad range of materials, including ferroic crystals [1], iron based superconductors [2], nano – confined molecular glass forming liquids [3] and polymers [4] and show the wealth of information (e.g. on domain wall motion dynamics, nematic precursor fluctuations, confinement effects at liquid – glass transitions, etc.) that can be extracted from measurements of their low frequency elastic response. Acknowledgement: The work was supported by the Austrian Science Fund (FWF) P23982-N20.

A distribution of relaxation times results in a relaxation described by formulae more complex than a single decreasing exponential function. A known example is the stretched exponential function [1] often treated as a continuous linear combination of purely exponential decays [2]. An experiment providing the relaxation function and the appropriate impulse response, i.e. the response of the system to the Dirac’s delta-like perturbation would be an evidence of a multiscale origin of the phenomenon. On the other hand, a non-exponential decay may result from a relaxation of a single anharmonic element without any recourse to different time scales. The amplitude-dependent response functions will be presented and the selected experimental data will be analyzed with both methods of description. Criteria will be proposed to distinguish the multiscale and non-linear [3] mechanisms of non-exponential decay. A sonic effect of reverberation with continuous and discrete distribution of relaxation times will be used to demonstrate how the ordinary exponential and non-exponential regimes affect the intelligibility of speech and music.

[2] see e.g. M.N. Berberan-Santos, E.N. Bodunov, B. Valeur. Chemical Physics 315 (2005), 171
I will discuss some general aspects of structural and magnetic correlations that can be accessed by neutron and x ray scattering techniques at low angle. Among several emergent systems investigated, I will focus on an exchanged coupled prototypical system under various conditions of field cooling. These studies show that magnetism in magnetic multilayers can be engineered without involving the microstructure of the individual layers. Some important correlations aspects will also be discussed with respect to rare-earth/rare-earth systems. Probing the coherent scattering due to vertically correlated magnetic structures with off-specular polarized neutron scattering, we confirm the existence of magnetic vortex-like domains associated with magnetic helical ordering within the layers. The opportunity for fundamental chiral spintronics in unconventional systems will be thereby introduced. Lastly, I will briefly touch upon the possibility to use in situ neutron reflectometry in mapping self-diffusion.
Piezoelectricity in three-dimensional (3D) materials is a well known physical phenomenon with many applications ranging from medical imaging (ultrasound) to fuel injection in motorcar engines. In earlier work we have investigated by analytical methods piezoelectricity and phonon dispersions in 2D and in multilayer crystals [1],[2]. Here we extend this work by taking into account lattice anharmonicities. Starting from a 2D honeycomb ionic crystal structure with D$_{3h}$ symmetry we use a Hamiltonian which includes anharmonic couplings between in-plane lattice displacements and out-of-plane flexural modes [3]. Using methods of statistical mechanics we derive coupled equations for acoustic, optical and flexural dynamic response functions. The resonances of the correlation functions allow us to study temperature dependent phonon lineshifts and dampings. In the limit of long wavelengths and low frequencies we recover macroscopic equations for sound waves, electrical polarization and flexural motion. There the macroscopic quantities such as sound velocities, piezoelectric coefficients and bending rigidity are expressed in terms of atomistic parameters. Effects due to two-dimensionality are discussed. As specific materials we refer to hexagonal boron nitride and transition metal dichalcogenides.

The computation of the critical exponent eta characterizing the universal elastic behavior of crystalline membranes in the flat phase continues to represent challenges to theorists as well as computer simulators that manifest themselves in a considerable spread of numerical results for eta published in the literature. We provide additional insight into this problem [A.T. PRE 91, 022132 (2015)], that results from combining Wilson’s momentum shell renormalization-group method with the power of modern computer simulations based on a recent optimization [A.T. PRB 87, 104112 (2013)] of our Fourier Monte Carlo algorithm. We discuss the ideas and difficulties underlying this combined scheme and present a calculation of the renormalization-group flow of the effective two-dimensional Young modulus for momentum shells of different thickness. Extrapolation to thick shells allows us to produce results in reasonable agreement with those obtained by functional renormalization group or by Fourier Monte Carlo simulations in combination with finite-size scaling. Moreover, our method allows us to obtain for the the first time a numerical estimate for the value of the Wegner exponent omega that determines the leading correction to scaling. This in turn allows us to refine our numerical estimate for eta previously obtained from precise finite-size scaling data [2], and also sheds some light on the possible reasons for the dispersion of previously published numerical estimates for eta. In particular, for the solid case, our numerical estimate for eta is markedly smaller than that derived from other recent simulations, and we find clear evidence against “intrinsic ripples”, whose existence has been repeatedly claimed in the graphene-related literature.
Spectroscopical characterisation of high surface area carbons through a multitechnique approach

PIOVANO, Andrea 1; LAZZARINI, Andrea 2; LAMBERTI, Carlo 2; AGOSTINI, Giovanni 3; LEOFANTI, Giuseppe 4; PELLEGRINI, Riccardo 5; CROPPO, Elena 2
1 Institut Laue-Langevin (ILL), Grenoble, France; 2 University of Turin, Turin, Italy; 3 European Synchrotron Radiation Facility (ESRF), Grenoble, France; 4 Consultant, Milano, Italy; 5 Chimet SpA, Viciomaggio Arezzo, Italy

High surface area carbons are industrially relevant materials whose properties depend on morphology, texture and surface features. The detailed characterization of functional groups on the surface of this class of materials is a fundamental step for understanding their potential in a variety of applications. Unfortunately IR, the widely used laboratory spectroscopy method, is difficult to be applied on carbons due to the intrinsic strong absorption. We present here an multitechnique approach, based on the synergic combination of three vibrational spectroscopies: i) FT-IR diffuse reflectance spectroscopy (DRIFT), that, limiting the strong absorption of the transmitted light is effective in evidencing vibrations with change in the dipole; ii) back-scattering Raman spectroscopy, which is sensitive mostly to carbon bulk vibrational modes; iii) Inelastic Neutron Scattering (INS) that, eliminates the problem of radiation interaction and is sensitive to vibrations involving hydrogen including species, highly abundant on carbons surface. The three technique are applied to two classes of activated carbons, subjected to specific chemical treatments. The whole set of experimental data, interpreted with the help of DFT calculations, allow us to point out their structural and surface properties, and to clarify some controversial information present in the specialized literature, where conclusions are done on the basis of the data obtained by a single technique.
Materials under high pressure

(De)formation of mantle minerals: Insights from atomic-scale simulations

JAHN, Sandro 1
1 Universität zu Köln, Cologne, Germany

Corresponding Author: s.jahn@uni-koeln.de

Minerals are the building blocks of the Earth. Knowledge of their formation and evolution is needed to understand both the structure and the dynamics of our planet. As only the upper part of the crust is accessible to direct sampling, models of the deep interior of the Earth rely on a combination of geophysical observations, laboratory experiments and simulations. Here, we use various atomic scale simulation methods to shed light on the structure and thermodynamic stability of mantle minerals, defects in their crystal structure and on the mechanisms of diffusion and shear deformation. These simulation techniques are unique in the sense that they provide simultaneous access to atomic structures and to thermodynamic or transport properties. On the other hand, chemical and structural complexity of relevant Earth materials require both substantial computational resources and efficient though still accurate simulation methods. We therefore use a combination of classical and first-principles molecular modeling methods, accelerated dynamics techniques such as metadynamics and sometimes educated guess. A big challenge for future research will be to establish the link between the atomic and the continuum scale, especially for modeling one- or two-dimensional crystal defects and for modeling plastic deformation.
Lattice dynamics and magnetic order in CrAs under pressure

WEHINGER, Björn 1,2; KELLER, Lukas 2; RÜEGG, Christian 2
1 University of Geneva, Geneva, Switzerland; 2 Paul Scherrer Institut (PSI), Villigen, Switzerland

Corresponding Author: bjorn.wehinger@unige.ch

Pressure induced superconductivity in CrAs has been discovered in June 2014, opening a new avenue for searching novel superconductors in Cr and other transition based compounds [1,2]. CrAs belongs to the group of 3d electron systems which can offer stages which induce intriguing superconductivity as realized in cuprates, Fe pnictides, cobalt oxyhydrate, etc. In Cr- and Mn-based systems this behaviour has so far not been observed. The application of external pressure, however, leads to superconductivity in CrAs in the vicinity of antiferromagnetic order. CrAs is paramagnetic at room temperature and shows a first order magnetic phase transition at 265 K to a helimagnetic phase. The magnetic transition is suppressed at higher pressures where superconductivity appears in the paramagnetic phase at low temperature. In order to investigate the origin of superconductivity in CrAs we perform neutron diffraction to study the magnetic structure under pressure [3], inelastic x-ray scattering to determine the phonon dispersion relations and ab initio calculations to address spin-lattice coupling.

In proper ferroelectrics, the large dielectric anomaly observed at Curie temperature $T_c$ is caused by softening of some polar excitation. In displacive ferroelectrics, this excitation is a polar phonon active in far-infrared spectra. In order-disorder ferroelectrics, dielectric relaxation with frequency in the MHz-GHz region drives the ferroelectric phase transition. Many ferroelectrics exhibit crossover from displacive to order-disorder type of phase transition, i.e. some phonon softens on cooling far above $T_c$, but additional relaxation (called central mode) appears close to $T_c$ and its relaxation frequency remarkably softens towards $T_c$. As examples we will present phonon and central mode behavior near strain-induced ferroelectric phase transitions in EuTiO$_3$ and Sr$_{n+1}$Ti$_n$O$_{3n+1}$ (n=1-6) thin films,[1-3] in relaxor ferroelectric Na$_{0.5}$Bi$_{0.5}$TiO$_3$ [4] and multiferroic PbFe$_{1/2}$Nb$_{1/2}$O$_3$.[5]

In multiferroics, where the ferroelectricity is induced by a spin order, only a small and narrow peak in temperature dependent permittivity appears at $T_c$. We will show that this tiny dielectric anomaly is caused by softening of an electromagnon, whose frequency lies in the microwave region. This electrically active spin excitation can have relaxation character in dielectric spectra (e.g. in MnWO$_4$) [6] or resonance character (e.g. in Sr$_3$Co$_2$Fe$_2$O$_{11}$ with Z-type hexaferrite structure).[7]

Germanium telluride (GeTe) has attracted an intense renewed interest in the past few years for its relevance and high performance as a phase-change material as such and in combination of the form (GeTe)m(Sb2Te3)n which find useful applications in modern non-volatile data storage devices. Apart from this technological interest, there is a very fundamental issue regarding whether the ferroelectric-to-paraelectric phase transition in GeTe is order-disorder or displacive in its origin. Also, the underlying physics of the crystal volume contraction which assists the structural transformation in GeTe remains far from clear.

Our contribution presents results of the high-resolution neutron powder diffraction experiments performed on a spallation neutron source which allow for a better understanding of the structural changes across the rhombohedral-to-cubic phase transition in GeTe. We also report on the phonon dynamics in GeTe which we gain from the inelastic neutron scattering experiments along with the density functional theory calculations that show conclusively the displacive type of the phase transition rather than the order-disorder one suggested by some x-ray absorption fine structure experiments and the pair-distribution function analysis. The structural phase transition in GeTe is shown to be driven by the condensation of exactly three components of the triply degenerate optical transverse soft-phonon mode at the Brillouin zone center. Results of the current work indicate that the local atomic potentials are single-well which strongly supports the displacive nature of the phase change in crystalline GeTe. Our considerations are relevant not only for GeTe but can be applicable to other ferroelectric materials like barium titanate as well as manganites showing colossal magnetoresistance, e.g., lanthanum manganite which are known to exhibit similar phenomena.
Multiferroics and ferroelectrics

Directional anisotropy of light in multiferroics

PIMENOV, Andrei

Vienna University of Technology, Vienna, Austria

Corresponding Author: pimenov@ifp.tuwien.ac.at

Multiferroics are materials which exhibit electric and magnetic order simultaneously. Due to the coupling of electric and magnetic effects, these materials show a strong potential to control electricity and magnetism and, more generally, the properties and propagation of light. One of the most fascinating and counter-intuitive recent results in multiferroics is directional anisotropy, the asymmetry of light propagation with respect to the direction of propagation. The absorption in the material can be different for forward and backward propagation of light, which in extreme case may lead to complete suppression of absorption in one direction. Another remarkable effect in multiferroics is directional birefringence, i.e. different velocities of light for different directions of propagation. As an example, in the multiferroic samarium ferroborate giant directional birefringence can be realized. The effect is easily observed for linear polarization of light in the range of millimeter-wavelengths, and survives down to very low frequencies. The dispersion and absorption close to the electromagnon resonance can be controlled and fully suppressed in one direction. Therefore, samarium ferroborate is a universal tool for optical control: with a magnetic field as an external parameter it allows switching between two functionalities: polarization rotation and directional anisotropy.
Tiny cause with huge impact: polar instability through strong magneto-electric-elastic coupling in bulk EuTiO$_3$

BUSSMANN-HOLDER, Annette $^1$; REUVEKAMP, Patrick $^1$; CASLIN, Kevin $^1$; KREMER, Reinhard $^1$; KÖHLER, Jürgen $^1$

$^1$ Max-Planck-Institute for Solid State Research, Stuttgart Germany

Corresponding Author: a.bussmann-holder@fkf.mpg.de

Multiferroic materials with combined polar, magnetic, and elastic orderings are at the forefront of scientific research in view of their multiple interactive couplings. Even though the phenomenon of multiferroicity has been predicted long ago [1], its realization remains rare since polar order is achieved when a transition metal d$^0$ configuration is combined with highly polarizable anions, whereas magnetic order relies on a finite d$^n$ configuration. These two requirements yield a certain incompatibility. Even though a rather large number of materials have been shown to exhibit the desired properties, the coupling between magnetic and polar order is either very weak, or the spontaneous polarization/magnetization appears at low temperature only and remains too small to be of technological interest. Here we propose a new strategy to achieve strong magnetic-polar coupling by deriving the soft mode frequency of EuTiO$_3$ as a function of its lattice parameters which exhibits unusual, yet very small temperature dependencies at high and low temperatures [2, 3]. Specifically we develop a route of how to induce ferroelectric order in bulk EuTiO$_3$ (ETO) by combining experimental results with theoretical concepts. We show that marginal changes in the lattice parameter of the order of 0.01% have a more than 1000% effect on the transverse optic soft mode of ETO and thus easily induce a ferroelectric instability.


Multiferroic RMn$_2$O$_5$ (R = Y, Tb, Ho) and isotopically substituted TbMn$^{16/18}$O$_3$, Dy$^{16/18}$MnO$_3$: A comprehensive Raman light scattering and neutron scattering investigation

Corresponding Author: c.ulrich@unsw.edu.au

Multiferroic materials demonstrate excellent potential for next-generation multifunctional devices, as they exhibit coexisting ferroelectric and magnetic orders. At present, the underlying physics of the magnetoelectric coupling is not fully understood, and competing theories exist with partly conflicting predictions. Therefore, we have investigated isotopically substituted TbMn$^{16/18}$O$_3$, Dy$^{16/18}$MnO$_3$, and RMn$_2$O$_5$ (R = magnetic Tb, Ho and non-magnetic Y) by Raman light scattering and neutron diffraction to elucidate the spin-phonon coupling and crystallographic as well as magnetic phase diagrams in order to shine light on the multiferroic coupling mechanism in both compounds.

Raman light scattering allows for the detection of subtle changes in phonon energy and lifetime at magnetic and ferroelectric phase transitions through interactions of the lattice vibrations with the electronic systems. This offers valuable information on the mechanisms behind the magnetoelectric properties. For example, our experiments on RMn$_2$O$_5$ did demonstrate that the magnetic and ferroelectric phases in RMn$_2$O$_5$ with magnetic R = Tb, Ho are distinct from the phases in non-magnetic YMn$_2$O$_5$, demonstrating the importance of the rare earth element on the multiferroic properties.

Our neutron diffraction investigations did yield additional complementary information in the crystallographic and magnetic structures. Our combined neutron and high resolution X-ray synchrotron investigation on Dy$^{16/18}$MnO$_3$ did allow for the detection of atomic displacements at the ferroelectric phase transition, possible responsible for the creation of the ferroelectric moment. Opposite to the behavior in other transition metal oxides, oxygen isotope substitution only had a minor effect on the magnetic properties. This provides valuable information on effects behind the magnetoelectric coupling mechanisms in these multiferroic materials.
Multiferroics and ferroelectrics

Dynamics of Nanoscale Polarization Fluctuations in a Uniaxial Relaxor

ONDREJKOVIČ, Petr 1; KEMPA, Martin 1; HLINKA, Jiří 1; KULDA, Jiří 2; FRICK, Bernhard 2; APPEL, Markus 2; COMBET, Jérôme 2; DEC, Jan 2; ŁUKASIEWICZ, Tadeusz 4
1 Academy of Sciences of the Czech Republic (AS CR), Prague, Czech Republic; 2 Institut Laue-Langevin (ILL), Grenoble, France; 3 University of Silesia, Katowice, Poland; 4 Institute of Electronic Materials Technology, Warsaw, Poland

Corresponding Author: ondrejkovic@fzu.cz

One of the most remarkable properties of relaxor materials is their extraordinarily large dielectric permittivity appearing over a broad temperature interval and attaining its maximum at a temperature $T_{\text{max}}$, which varies linearly with the logarithm of the probing frequency. This frequency-dependent $T_{\text{max}}$ is described by the Vogel-Fulcher (VF) law and originates from a temperature-dependent dielectric relaxation. Such a behaviour has also been observed in tetragonal tungsten bronze crystals such as Sr$_{0.61}$Ba$_{0.39}$Nb$_2$O$_6$ (SBN61) [1], an almost ideal uniaxial relaxor with polar fluctuations appearing only along the tetragonal axis. Recently, we have performed a neutron backscattering study on a SBN61 single crystal in the MHz-GHz frequency region [2]. Investigation of diffuse scattering coming from atomic displacements along the tetragonal axis allowed us to resolve the dynamic part of nano-scale polar fluctuations. Typical data are displayed in Fig.1a, showing a clear inelastic component which can be well described by a simple model based on an analysis of dielectric spectra [1,2]. The agreement between the experiment and model data can be better appreciated when the scattering intensity at a fixed energy transfer is plotted as a function of temperature (cf. Fig.1b,c). This comparison demonstrates that the peak positions shift towards higher temperatures with increasing energy transfers, closely following the VF law. Our results provide direct evidence that the ‘critical’ relaxation with its VF-type frequency dependence is associated with dynamic nano-scale polarization fluctuations.


Fig.1: Neutron-scattering intensity at $Q \sim (0.15,0,1)$ as a function of (a) energy transfer and (b) temperature compared with (c) a model based on an analysis of dielectric spectra [1,2].
The technique of dielectric spectroscopy which overlaps frequency range from 1 mHz to 5 THz is a powerful tool to investigate disordered materials. Such experiments can be combined with FTIR measurements in order to describe the dynamics of polar nanoregions and optical phonons in materials like relaxor ferroelectrics. In this contribution the broadband dielectric spectroscopy was employed to investigate several solid solution systems based on sodium bismuth titanate (i.e. 0.4Na0.5Bi0.5TiO3-(0.6-x)SrTiO3-xPbTiO3, (0.4-y)Na0.5Bi0.5TiO3-0.6SrTiO3-yPbTiO3 and zNa0.5Bi0.5TiO3-(1-z)Sr0.7Bi0.2TiO3). All three systems show rich behavior ranging from glassy state which crossovers to relaxor and even normal ferroelectric phase. The influence of polar nanoregions and phase diagrams of investigated materials will be discussed. In addition, ferroelectric hysteresis, pyroelectric and piezo measurements will be presented.
Ab initio vibrational properties of the MXene materials functionalized by fluorine, oxygen and hydroxyl group

WASIK, Magdalena 1; WDOWIK, Urszula 1
1 Pedagogical University of Cracow, Cracow, Poland

Corresponding Author: mmedala@up.krakow.pl
A new family of 2D-like nano-sized binary and ternary transition metal carbides (known also as MXenes) has received significant scientific interest due to their intriguing functionalities and technological applications. Physical and chemical properties of these material can be triggered by terminating their surfaces by various adatoms or molecules. This contribution presents first-principle studies of the influence of fluorine and oxygen adatoms as well as the surface terminating OH group on the lattice dynamics of pristine Ti2C monolayers.
Reflection, refraction, mode conversion and guided waves on surfaces and interfaces of materials with all allowed Poisson ratios

Corresponding Author: pawel.sobieszczyk@ifj.edu.pl

When encountering a mismatch of characteristic impedance a bulk acoustic wave transforms into up to three reflected and refracted waves of different polarizations. The effect is known as mode conversion [1]. The lack of the specularly reflected wave is called total mode conversion because then all the outgoing waves propagate at speeds different than that of the incident one. Conversely, if the only outgoing wave reflects in the specular way one speaks of no-conversion. Discovery of materials with negative Poisson’s ratio [2] enlarged the range of possible impedance mismatch. The conditions for the total mode conversion, for no-conversion and for evanescent partial waves will be presented for half-space elastic media and for interfaces between two different elastic media also separated by a thin membrane. Some frequencies corresponding to these phenomena turn out to coincide with apparently spurious roots of the secular determinant giving, in principle, the frequencies of the surface or interface waves [3,4]. These results will be compared with the anomalies of local densities of states (LDOS). Of particular interest are maxima of and minima of LDOS corresponding to surface resonances and surface antiresonances respectively. Some sharp surface resonances mark the total mode conversion of bulk waves and broader resonances an analogous mode conversion of evanescent waves. The effects of curved surfaces will be also summarized [5].

Effects of $^{18}$O isotope substitution in multiferroic RMnO$_3$ (R=Tb, Dy)

GRAHAM, P.J. 1; NARAYANAN, N. 2; MCINTYRE, G. J. 3; HUTCHINSON, W. 1; Prof. ULRICH, C. 1; REYNOLDS, N. 1; ROVILLAIN, P. 1; HESTER, J. 3; KIMPTON, J. 3; YETHIRAJ, M. 3; POMJAKUSHINA, E. 7; CONDER, K. 7; KENZELMANN, M. 4

1 University of New South Wales, Sydney, Australia; 2 UNSW Canberra, Canberra, Australia; 3 The Australian Synchrotron, Australian Nuclear Science and Technology Organisation, Melbourne, Australia; 4 Paul Scherrer Institut (PSI), Villigen, Switzerland

Corresponding Author: p.j.graham@unsw.edu.au

Multiferroic materials demonstrate desirable attributes for next-generation multifunctional devices as they exhibit coexisting ferroelectric and magnetic orders. In type-II multiferroics, coupling exists that allows ferroelectricity to be manipulated via magnetic order and vice versa, offering potential in high-density information storage and sensor applications. Despite extensive investigations into the subject, questions of the physics of magnetoelectric coupling in multiferroics remain, and competing theories propose different mechanisms. The aim of this investigation was to study changes in the statics and dynamics of structural, ferroelectric and magnetic orders with oxygen-18 isotope substitution to shine light into the coupling mechanism in multiferroic RMnO$_3$ (R=Tb, Dy) systems. We have performed Raman spectroscopy on $^{16}$O and $^{18}$O-substituted TbMnO$_3$ single crystals. Oxygen-18 isotope substitution reduces all phonon frequencies significantly. However, specific heat measurements determine no changes in Mn$^{3+}$ (28 and 41 K) magnetic phase transition temperatures. Pronounced anomalies in peak position and linewidth at the magnetic and ferroelectric phase transitions. While the anomalies at the sinusoidal magnetic phase transition (41 K) are in accordance to the theory of spin-phonon coupling, further deviations develop upon entering the ferroelectric phase (28 K). Furthermore, neutron diffraction measurements on $^{16}$O and $^{18}$O-substituted DyMnO$_3$ powders show structural deviations at the ferroelectric phase transition (17 K) in the order of 100 fm. These results indicate that structure is actively involved in the emergence of ferroelectricity in these materials.
Recently, a new type of porous materials called coordination polymers or metal-organic frameworks (MOFs) emerged and attracted attention of the scientific community. These crystalline compounds are unique due to the highly porous structures which can be utilized for gas adsorption related applications. Some of MOF materials contain paramagnetic transition-metal ions, resulting in peculiar magnetic properties of these compounds. In addition, the organic part in some coordination polymers consists of polar molecules, which below a certain phase transition temperature order into a ferroelectric phase. Lately, a promising MOF [(CH$_3$)$_2$NH$_2$][Zn(HCOO)$_3$] with perovskite-type architecture and inherent ferroelectricity was synthesized. It is believed that the ferroelectric phase in this material is due to the ordering of (CH$_3$)$_2$NH$_2^+$ ions, but, however, the precise phase transition mechanism is still obscure. In this work we investigate the [(CH$_3$)$_2$NH$_2$][Zn(HCOO)$_3$] MOF doped with 0.05 mol % paramagnetic Mn$^{2+}$ ions using the continuous-wave (CW) and pulsed EPR methods. The temperature dependent X-band CW and field-sweep as well as Q-band CW EPR spectra reveal that the local Mn$^{2+}$ ion-probes are indeed sensitive to the local structural changes occurring at the phase transition point. Spectral simulations were used to obtain the g, hyperfine A and fine-structure D tensors and temperature dependence of their components allowing to further characterize the observed phase transition and the MOF structure. Following the temperature dependence of the axial zero-field splitting parameter D, it was concluded that the phase transition into the ferroelectric phase is of the first order.
Corresponding Author: kempa@fzu.cz

Piezoelectric crystals of the Pb(Fe_{1/2}Nb_{1/2})_{1-x}Ti_{x}O_{3} (PFN-xPT) system have drawn much interest in recent years, due to relatively high Curie temperatures and potential multi-ferroic properties. By substitution of Fe^{3+}/Nb^{5+} by Ti^{4+}, the magnetic properties are suppressed: the Néel temperature $T_{N}$ decreases rapidly with the Ti content and the Curie temperature $T_{C}$ increases almost linearly. Moreover, at about $x \approx 0.12$, PFN-xPT possesses a morphotropic phase boundary (MPB) between the monoclinic and tetragonal ferroelectric phases. Recently, a polarized Raman study [1] of the PFN-38 %PT single crystal reported significant crystalline anisotropy similar to that of tetragonal PbTiO$_{3}$. In this contribution, we will present our inelastic-neutron-scattering results of lattice dynamics of the PFN-38 %PT single crystal in the cubic and tetragonal phases, mainly with respect to the temperature behaviour of the TO soft mode around the phase transition, and the TA-TO coupled-mode analysis in different Brillouin zones and directions. Further the comparison with the end-members of the PFN-xPT series, pure PbTiO$_{3}$ [2-5] and Pb(Fe_{1/2}Nb_{1/2}) [6], will be discussed.

Elastic constants in multiferroic $\text{Bi}_2\text{Mn}_4\text{O}_{10}$

ZIEGLER, Fabian; GIBHARDT, Holger; SOBOLEV, Oleg; MURSHED, Mangir; GESING, Thorsten; ECKOLD, Götz

1 Georg-August-Universität Göttingen, Göttingen, Germany; 2 Universität Bremen, Bremen, Germany

Corresponding Author: ziegle@gwdg.de

Mullite-type $\text{Bi}_2\text{Mn}_4\text{O}_{10}$ [1] is an example for a multiferroic compound with a Néel temperature of 39 K, although its crystal structure [2] is not typical for allowing ferroelectricity. The dipoles of the constituent $\text{Mn}^{4+}\text{O}_6$ (along c-axis, bond valence sum BVS = 3.90(2) v.u.) and $\text{Mn}^{3+}\text{O}_5$ (along b-axis, BVS = 3.04(2) v.u.) polyhedra are oriented in different directions [3]. Both its nuclear and magnetic structural features differ from those of other rare-earth members of the $\text{R}_2\text{Mn}_4\text{O}_{10}$ family. While each member of $\text{R}_2\text{Mn}_4\text{O}_{10}$ family possesses incommensurate magnetic character [4], $\text{Bi}_2\text{Mn}_4\text{O}_{10}$ exhibits a commensurate [5] magnetic structure. In order to characterize its lattice dynamical properties we have studied the acoustic phonon branches of a single crystal of $\text{Bi}_2\text{Mn}_4\text{O}_{10}$ at room temperature using inelastic neutron scattering (INS). Experiments have been performed at the three-axes spectrometer PUMA@FRM II. The dispersion curves of the acoustic phonon branches in the Brillouin zone have been measured for different propagation directions close to the zone center (Gamma-point) and for different polarization vectors. The linear slopes of the corresponding dispersion curves are related to a specific combination of the elastic constants $c_{ij}$. We were able to determine the complete set of nine elastic constants $c_{ij}$ provided by the orthorhombic crystal (Pbam). The results clearly demonstrate the pronounced mechanical anisotropy of $\text{Bi}_2\text{Mn}_4\text{O}_{10}$.

Analytic approach to anharmonic modes of lattice vibrations.

JOCHYM, Paweł T. 1; WEHINGER, Björn 2
1 Institute of Nuclear Physics, Polish Academy of Science, Cracow, Poland; 2 University of Geneva, Geneva, Switzerland; Paul Scherrer Institut (PSI), Villigen, Switzerland

Corresponding Author: pawel.jochym@ifj.edu.pl

The classical theory of lattice dynamics deals with harmonic crystals. While this theory is very effective with describing large number of physical phenomena connected with lattice vibrations, it leaves out an important aspect of the lattice dynamics: anharmonic effects. Without this component many important physical phenomena cannot be properly described: thermal expansion, phase transitions, thermal equilibrium, thermal conductivity, multi-phonon processes - to name just a few. Over the years a number of effective methods have been developed to deal with cases where the anharmonicity could be treated as a small perturbation in the harmonic model. In many situations this approach is useful and effective (e.g. Quasi Harmonic Approximation for dealing with thermal expansion). Unfortunately, in cases where forces in the crystal are strongly anharmonic (e.g. phase transitions, phonon modes with strongly anharmonic potentials) this approach is much less effective.

In crystals the anharmonic component may take various forms. In many materials (e.g. PbTe, TiO₂) one or more of vibrational modes is characterized by a strongly anharmonic potential of the general form of the fourth order polynomial. The equation of motion in such a potential can be solved analytically and the result can be further analysed to obtain experimentally verifiable properties: mode frequency as a function of temperature, thermal displacements, line profile etc. Even in cases where the potential does not allow for analytical solution, the procedure can still be carried out, however with higher computational cost, using numerical integration of the equation of motion.

This work presents a computational scheme for this type of calculation and demonstrates the derivation of temperature dependence of phonon frequency in the case of anharmonic mode in rutile titanium dioxide. The calculation is based on the DFT-derived potential for the mode.
Effect of CFO and PZT fillers on Dielectric and Ultrasonic Properties of P(VDF-TrFE) Copolymer Based Composites

SAMULIONIS, Vytautas 1; JAROSLAVAS, Belovickis 1; SVIRSKAS, Šarūnas 1; IVANOV, Maksim 1; BANYS, Jūras 1; SILIBIN, Maksim 2; LANCEROS-MÉNDEZ, Senentxu 3

1 Vilnius University, Vilnius, Lithuania; 2 National Research University of Electronic Technology, Moscow, Russia; 3 University of Minho, Braga, Portugal

Corresponding Author: jaroslavas.belovickis@ff.vu.lt

Composites are considered to be any multiphase materials that show a combination of properties of their components. PZT, CoFe₂O₄ and BaTiO₃ are one of ingredients that can improve the dielectric properties and the ultrasonic properties of polymer based composites. In this work we report on both the dielectric and the ultrasonic properties of the conventional polymer polyvinylidene fluoride / trifluoroethylene (P(VDF-TrFE)) of the composition 70/30 mol % with various concentrations of (Pb₇₅Ba₂₄Sr₀₁)(Zr₅₃Ti₄₇)O₃ (BPZT) and CoFe₂O₄ (CFO) fillers. By the means of dielectric spectroscopy it is shown that the dielectric properties may be tuned by varying the volume fraction of the ferroelectric fillers. The dependencies of the dielectric properties of the composites on filler volume fraction are reported and analyzed in terms of an analytical model (Lichteneker’s effective medium approximation) applying electrodynamic boundary conditions. Experimental study of ultrasonic wave attenuation, velocity and piezoresponse in these composites has been performed over wide temperature range (100 K – 410 K) using ultrasonic automatic pulse-echo technique. The temperature dependences of ultrasonic velocity and attenuation showed anomalies attributed to the glass transition and paraelectric-ferroelectric phase transition. Above Curie temperature $T_c$ the piezoresponse vanishes in beforehand polarized samples.
Order by disorder or energetic selection of the ground state in the XY pyrochlore antiferromagnet \( \text{Er}_2\text{Ti}_2\text{O}_7 \)? A neutron scattering study.

PETIT, Sylvain 1; ROBERT, Julien 2; BONVILLE, Pierre 1; OLLIVIER, Jacques 2; MUTKA, Hannu 4; DECORSE, Claudia 5; MIREBEAU, Isabelle 5; GUITTENY, Solène 1; GINGRAS, Michel 6

1 CEA, Centre de Saclay, Gif sur Yvette, France; Laboratoire Léon Brillouin (LLB), Gif sur Yvette, France; 2 CNRS, Grenoble, France; 3 CNRS, Centre de Saclay, Gif sur Yvette, France; 4 Institut Laue-Langevin (ILL), Grenoble, France; 5 Université Paris XI, Paris, France; 6 University of Waterloo, Waterloo, Canada

Examples of materials where an “order by quantum disorder” mechanism is at play to select a particular ground state are scarce [1,2]. It has been recently proposed that the anti-ferromagnetic pyrochlore \( \text{Er}_2\text{Ti}_2\text{O}_7 \) reveals a most convincing case of this mechanism [3,4,5]. Observation of a spin gap at zone centers was interpreted as a definitive proof of this physics [6]. We argue, however, that the magnetic anisotropy provided by the interaction-induced admixing between the CEF ground and excited levels gives an alternative energetic mechanism [7,8]. RPA calculations based on a mean field model taking into account explicitly the CEF anisotropy reproduce well new high resolution inelastic neutron scattering data. Here, the gap originates from the anisotropy rather than quantum fluctuations effects. The present study raises the question of the quantum order by disorder as the sole or even principal mechanism for the selection of the magnetic ground state in this material.

Guided surface waves on interfaces of media with positive and negative Poisson’s ratio

KUŹMA, Dominika 1; SOBIESZCZYK, Paweł 1; MAJKA, Marcin 1; ZIELIŃSKI, Piotr 1
1 Institute of Nuclear Physics, Polish Academy of Science, Cracow, Poland

Corresponding Author: dominika.kuzma@ifj.edu.pl
Surfaces and interfaces are waveguides for some kinds of waves. The Stoneley wave occurs on the interface of perfectly bonded isotropic elastic materials [1]. The kind of waves are of importance e.g. in geoscience [2] and in the design of delay lines in acoustical waveguides [3]. Whereas the surface Rayleigh wave exists on all free surfaces of elastic media, the range of existence of the Stoneley waves is rather narrow. It will be shown how the use of auxetics, i.e. the materials with negative Poisson’s ratio [4] enlarges this region. Qualitatively new guided waves arise if the media are separated by an interlayer. The case of a thin membrane will be discussed with an emphasis on long wavelength cut-offs. The systems under consideration admit a number of evanescent waves known as surface resonances or surface leaky waves [5].

Electric control of the unidirectional transmission in the ferrotoroidic LiCoPO$_4$

KOCIS, Vilmos 1; KÉZSMÁRKI, István 1; TOKUNAGA, Yusuke 2; RÕÕM, Toomas 3; NAGEL, Urmas 3; BORDÁCS, Sándor 1; TOKURA, Yoshinori 2; TAGUCHI, Yasujiro 2

1 Budapest University of Technology and Economics, Budapest, Hungary; 2 RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama, Japan; 3 National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

Corresponding Author: vilmos.kocsis@gmail.com

Multiferroics allow the magnetic control of electric polarization and the electric control of magnetization via the static magnetoelastic effect (ME). Dynamic or optical ME effects gained high interest because they give rise to unidirectional transmission - as recently observed in low-temperature multiferroics. This phenomenon allows the development of optical diodes, which transmit unpolarized light in one, but not in the opposite direction. Ferroelectric polarization and spontaneous magnetization in multiferroics can be exploited to switch the transmission direction with either magnetic or electric field as shown in Fig. 1. In prior optical directional effects in solids were only investigated with magnetic field, but were never tested in the presence of external electric field before. LiCoPO$_4$ is a well known multiferroic material with an exotic, recently discovered degree of freedom known as toroidal moment [4]. Neutron diffraction and magnetization studies have revealed complex magnetic phases in both compounds pointing to the existence of several competing energy scales. The exotic magnetic interactions and the possible finite macroscopic toroidal moment of this material promote it to an ideal candidate for novel optical magnetoelastic experiments. By means of far-infrared absorption measurements we have revealed the existence of unidirectional transmission which could be controlled by either magnetic or electric fields (Fig. 1). The samples were cooled down to the antiferromagnetically ordered phase in crossed electric and magnetic fields and the measurements were performed in the presence of these static fields.

Figure 1: Schematic representation of the optical diode function in multiferroics (left) and electric control of unidirectional transmission at the spin-wave resonances of LiCoPO$_4$. 
Dynamics of water confined in chrysotile asbestos studied by inelastic neutron scattering

IVANOV, Alexandre 1; KOLESNIKOV, Alexander 2; EGAMI, Takeshi 3; VAKHRUSHEV, Sergey 4,5; ANDRONIKOVA, Daria 4; LOKSHIN, Konstantin 3; KUMZEROV, Yuri 4; FILIMONOV, Alexey 4,5

1 Institut Laue-Langevin (ILL), Grenoble, France; 2 Oak Ridge National Laboratory, Oak Ridge, USA; 3 Joint Institute for Neutron Sciences, Oak Ridge National Laboratory, Oak Ridge, USA; University of Tennessee, Knoxville, USA; 4 Ioffe Physical-Technical Institute, St. Petersburg, Russia; 5 St. Petersburg State Polytechnical University, St. Petersburg, Russia

Corresponding Author: aivanov@ill.fr

We report the new data on the molecular dynamics of water confined in the "channels" of the chrysotile asbestos structure obtained by neutron spectroscopy. The neutron scattering measurements have been carried out on the time-of-flight spectrometer Sequoia at SNS (Oak Ridge, USA). The energy range up to 600 meV was covered with the instrument conditions selected to emphasize different parts of the full range of water vibration dynamics. The neutron spectra of the dry and wet samples were recorded at the identical conditions and the difference spectra were obtained by subtracting the 'dry' spectra from the 'wet' ones. Special care was taken to keep the preferred orientation of the fibers (c-axis) in the samples so that the resulting misorientation of the channels does not exceed ±12.5 degrees from a selected direction. The neutron scattering measurements were performed with the two sample geometries: with the channel axes along the neutron wave vector transfer Q in the scattering plane and perpendicular to the scattering plane. This permitted us to track the preferred direction of the hydrogen vibrations corresponding to different spectra ranges: acoustic, librational, molecular frequencies.

We have found evidences for particularly strong anisotropy of confined water vibrations in the libration band (50-130 meV) which appears to be split onto 3 peaks. Such sharp peaks different bulk-ice phases were observed so far only in the inelastic neutron scattering spectra of the proton ordered phases (ice-II, ice-VIII and partially ordered ice-VI) while the proton disordered phases exhibit in this range practically featureless spectra, similar to that of ice-Ih. These observations have been confirmed in the measurements of deuterated water in the protonated asbestos what permitted us to move out from the range of strong vibration bands observed in the asbestos itself.
Recently, we have studied dielectric spectroscopy of variously conducting polyaniline (PANI) pellets in a very broad frequency ($10^{-2}$–$10^{13}$ Hz) and temperature ($10$–$300$ K) range [1]. The DC conductivity varied between $\approx 10$ S/cm for the emeraldine salt and $\approx 10^{-12}$ S/cm for the deprotonated emeraldine, the PANI base. Mechanism of the conduction consists of polaron transfer along the PANI chains and the reason for such dramatic differences is a result of various degrees of disorder within the chains and their arrangement [2]. Since the fully ordered metallic PANI films with DC conductivity of $\approx 10^3$ S/cm were also reported [3], we attempted here to model the whole dielectric and conductivity spectrum of our emeraldine salt pellets as a nanocomposite of the metallic PANI and our amorphous PANI base. For modelling of the conductivity including the THz and infrared part with vibrational modes we have used the effective medium approach based on Bruggeman and generalised Lichtenecker model [1]. Both models are discussed from the view point of topology and percolation of the conductive fraction and preferences of the latter model are demonstrated.

In physical systems simultaneously breaking time-reversal and spatial inversion symmetries the strength of absorption for two counter-propagating light beams can be different irrespective of the polarization state of light [1], which phenomenon is termed as non-reciprocal directional dichroism. Until recent experiments on multiferroic materials [2, 3] this effect was generally found to be weak. Directional dichroism of multiferroics in the far-infrared spectral range is the consequence of the optical magnetoelectric effect, i.e. the coupled dynamics of spins and local electric dipoles [4]. Spin-wave modes in multiferroics can simultaneously be excited by the electric and magnetic components of light, hence, they can be viewed as the “elementary excitations” of such hybrid magnetoelectric response. Indeed multiferroic Ni₃TeO₆ [5] shows strong directional dichroism in its spin excitations, even for unpolarized light. The temperature- and magnetic field dependence of these resonances was followed up to the Néel temperature and up to 30 T, respectively.
Ab initio study of the strain-mode coupling in SrBi$_2$Nb$_2$O$_9$

PETRALANDA, Urko ¹; ETXEBARRIA, Iñigo ¹
¹ University of the Basque Country, Bilbao, Spain

Corresponding Author: inigo.etxebarria@ehu.eus

The Aurivillius compound SrBi$_2$Nb$_2$O$_9$ (SBN) has commonly been considered as a potential candidate for nonvolatile memories, and as a consequence, it has been thoroughly investigated both experimentally [1-3] and computationally [4,5]. The phase diagram of SBN is governed by three relevant distortions, and it has been shown that the trilinear coupling among them stabilizes the ferroelectric ground state [4-6]. An analogous critical influence of the trilinear coupling is also observed in the isomorphous SrBi$_2$Ta$_2$O$_9$ (SBT), where slight differences in the mode interplay induce the presence of an intermediate non-polar phase [3,5,6]. In this work we evaluate by ab initio calculations the couplings of the two components of the strain tensor that do not break the parent tetragonal symmetry with the three relevant symmetry adapted modes. We find that the three modes show significant couplings with strain. Elastic enthalpy is also calculated and we find that a particular combination of applied stress and misfit strain can be used to produce an enhancement of the spontaneous polarization as obtained in other materials [7].

Evolution of the helimagnon dispersion

WEBER, Tobias 1; GEORGII, Robert 1; BÖNI, Peter 1
1 Technische Universität München, Munich, Germany

Corresponding Author: tobias.weber@frm2.tum.de

We present measurements of the magnetic field-dependency of the helimagnetic band structure in MnSi. For low fields the helimagnons were previously discovered and mapped out by Janoschek et al. (Phys. Rev. B, 81(21), 214436, 2010) and Kugler et al. (arXiv:1502.06977, 2015), respectively. The high-field ferromagnetic dispersion, on the other hand, has been well known since the 1970s when it was measured by Ishikawa et al. (Phys. Rev. B, 16(11), 4956, 1977) Preliminary measurements we performed on the triple-axis spectrometer MACS (at NIST) suggest that the helimagnetic bands can still be seen even in the ferromagnetic regime (we used fields up to 1 T). This would still be in agreement with Ishikawa as they used thermal neutrons and thus had such a large resolution volume as to not being able to discern individual bands. Our measurements are currently being continued at the instruments MIRA (at MLZ) and later at TASP (at PSI). So far at MIRA we could see the band structure collapse into a single-magnon dispersion for very high fields of a few tesla. For fields below one tesla we saw a shifting in energy of mainly the first band. Here, the spectrum appears as a single non-symmetric peak as the first band moves towards the position of the other bands.
New multiferroic materials on the base of Co-doped barium titanate

BUJAKIEWICZ-KORONSKA, Renata 1
1 Pedagogical University of Cracow, Cracow, Poland

Corresponding Author: sfbujaki@cyf-kr.edu.pl
New ceramics (1-x)Ba_{0.95}Pb_{0.05}TiO_3-xCo_{0.10} (BPTC) were prepared by the conventional hot-sintering method in the aim of searching new multiferroic materials which could be very useful for the electronic industry. Substitution Pb^{2+} ions in A—site caused reduction of Curie temperature [1] and the smoothing of Young modulus in a wide range of temperatures. The addition of Co ions caused broadening of the dielectric anomalies related to the transition to the paraelectric cubic phase, and the structural transition between tetragonal and orthorhombic phases. Co impurities allowed the smoothing of the area of the phase transition by stabilization of the dielectric losses in the wide range of temperatures. The temperature dependence of the magnetic susceptibility \( \chi_{DC} \) were measured for BPTC-2.0, 5.0, 10.0 % in the ZFC and FC modes in the field of 50 kOe at 2 K. Ab initio simulations were processed in SIESTA 3.2 code together with spin polarization, GGA and LCAO with localized basis set. BPTC seems to be a multiferroic of I type with weak coupling between ferroelectric and magnetic properties.

Acknowledgments
The authors acknowledge the CPU time allocation at Academic Computer Centre CYFRONET AGH in Cracow. This work was supported in part by PL-Grid Infrastructure.

The cold three-axis neutron spectrometer at MLZ was designed for high-resolution, high flux with notable low background experiments under extreme conditions like high field and very low temperatures. The idea to provide overlap to thermal wavelengths was thought to give opportunity to extend typical cold-wavelength experiments to higher energy transfers keeping experimental conditions unchanged (see Fig. 1). Being in operation since 2005, many experiments have been performed on PANDA at energy transfers up to 10...12 meV by need of higher resolution than thermal TAS can provide. The further development of PANDA will respect the topic of cold TAS as well as the thermal overlap: First, the application of focusing optics is studied to investigate small samples or pressure dependent magnetic properties. Secondly, a multi-analyzer-multi-detector option called BAMBUS is just under design.

**Fig. 1**: Temperature dependence of high and low energy part of the excitation spectrum in superconducting FeSe$_x$Te$_{1-x}$ (x = 0.4) measured on PANDA by S. Li et al., PRL 105 157002 (2010)
<table>
<thead>
<tr>
<th>Name</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agostinho Moreira, J.</td>
<td>29</td>
</tr>
<tr>
<td>Agostini, G.</td>
<td>83</td>
</tr>
<tr>
<td>Almeida, A.</td>
<td>29</td>
</tr>
<tr>
<td>Andronikova, D.</td>
<td>125</td>
</tr>
<tr>
<td>Appel, M.</td>
<td>99</td>
</tr>
<tr>
<td>Argyriou, D.</td>
<td>97</td>
</tr>
<tr>
<td>Artyukhin, S.</td>
<td>129</td>
</tr>
<tr>
<td>Bahn, E.</td>
<td>43</td>
</tr>
<tr>
<td>Banys, J.</td>
<td>101, 109, 117</td>
</tr>
<tr>
<td>Becker, P.</td>
<td>25</td>
</tr>
<tr>
<td>Birks, E.</td>
<td>101</td>
</tr>
<tr>
<td>Bohaty, L.</td>
<td>25</td>
</tr>
<tr>
<td>Bönì, P.</td>
<td>133</td>
</tr>
<tr>
<td>Bonville, P.</td>
<td>71, 119</td>
</tr>
<tr>
<td>Bordács, S.</td>
<td>21, 123</td>
</tr>
<tr>
<td>Boris, A.</td>
<td>63</td>
</tr>
<tr>
<td>Bosak, A.</td>
<td>61</td>
</tr>
<tr>
<td>Brandlein, M.</td>
<td>67</td>
</tr>
<tr>
<td>Brubach, J-B.</td>
<td>27</td>
</tr>
<tr>
<td>Brückel, T.</td>
<td>137</td>
</tr>
<tr>
<td>Bujakiewicz-Koronska, R.</td>
<td>135</td>
</tr>
<tr>
<td>Bussmann-Holder, A.</td>
<td>95</td>
</tr>
<tr>
<td>Calvo-Almazan, I.</td>
<td>43</td>
</tr>
<tr>
<td>Caslin, K.</td>
<td>95</td>
</tr>
<tr>
<td>Čermák, P.</td>
<td>137</td>
</tr>
<tr>
<td>Chaix, L.</td>
<td>27</td>
</tr>
<tr>
<td>Chang, J.</td>
<td>65</td>
</tr>
<tr>
<td>Chatterji, T.</td>
<td>91</td>
</tr>
<tr>
<td>Cheong, S. W.</td>
<td>129</td>
</tr>
<tr>
<td>Chumakov, A.</td>
<td>13</td>
</tr>
<tr>
<td>Combat, J.</td>
<td>99</td>
</tr>
<tr>
<td>Conder, K.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Croppo, E.</td>
<td>83</td>
</tr>
<tr>
<td>Damay, F.</td>
<td>67</td>
</tr>
<tr>
<td>Daou, R.</td>
<td>67</td>
</tr>
<tr>
<td>De Brion, S.</td>
<td>27</td>
</tr>
<tr>
<td>Dec, J.</td>
<td>99</td>
</tr>
<tr>
<td>Decorse, C.</td>
<td>71, 119</td>
</tr>
<tr>
<td>Demmel, F.</td>
<td>43</td>
</tr>
<tr>
<td>Donner, W.</td>
<td>35</td>
</tr>
<tr>
<td>Dunce, M.</td>
<td>101</td>
</tr>
<tr>
<td>Eckold, G.</td>
<td>113</td>
</tr>
<tr>
<td>Egami, T.</td>
<td>125</td>
</tr>
<tr>
<td>Ehlers, D.</td>
<td>23</td>
</tr>
<tr>
<td>Elkaim, E.</td>
<td>67</td>
</tr>
<tr>
<td>Engelkamp, H.</td>
<td>129</td>
</tr>
<tr>
<td>Eng, L. M.</td>
<td>33</td>
</tr>
<tr>
<td>Ebebarria, I.</td>
<td>131</td>
</tr>
<tr>
<td>Evenson, Z.</td>
<td>39</td>
</tr>
<tr>
<td>Fabrèges, X.</td>
<td>27</td>
</tr>
<tr>
<td>Fauth, F.</td>
<td>67</td>
</tr>
<tr>
<td>Filimonov, A.</td>
<td>125</td>
</tr>
<tr>
<td>Forrest, T.</td>
<td>61</td>
</tr>
<tr>
<td>Fouquet, P.</td>
<td>43</td>
</tr>
<tr>
<td>Frick, B.</td>
<td>99</td>
</tr>
<tr>
<td>Fultz, B.</td>
<td>45</td>
</tr>
<tr>
<td>Georgii, R.</td>
<td>133</td>
</tr>
<tr>
<td>Gesing, T.</td>
<td>113</td>
</tr>
<tr>
<td>Gibhardt, H.</td>
<td>25, 113</td>
</tr>
<tr>
<td>Gingras, M.</td>
<td>119</td>
</tr>
<tr>
<td>Glensk, A.</td>
<td>49, 69</td>
</tr>
<tr>
<td>Goering, E.</td>
<td>47</td>
</tr>
<tr>
<td>Goian, V.</td>
<td>89</td>
</tr>
<tr>
<td>Grabowski, B.</td>
<td>49, 69</td>
</tr>
<tr>
<td>Graham, P. J.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Guitteny, S.</td>
<td>71, 119</td>
</tr>
<tr>
<td>Heid, R.</td>
<td>47</td>
</tr>
<tr>
<td>Hester, J.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Hickel, T.</td>
<td>49, 69</td>
</tr>
<tr>
<td>Hilinka, J.</td>
<td>51, 53, 99, 111</td>
</tr>
<tr>
<td>Hutchinson, W.</td>
<td>107</td>
</tr>
<tr>
<td>Hutchinson, W.</td>
<td>97</td>
</tr>
<tr>
<td>Ivanov, A.</td>
<td>35, 47, 125</td>
</tr>
<tr>
<td>Ivanov, M.</td>
<td>117</td>
</tr>
<tr>
<td>Jahn, S.</td>
<td>85</td>
</tr>
<tr>
<td>Jaroslavas, B.</td>
<td>117</td>
</tr>
<tr>
<td>Jochym, P. T.</td>
<td>115</td>
</tr>
<tr>
<td>Kamba, S.</td>
<td>89, 101</td>
</tr>
<tr>
<td>Kehr, S. C.</td>
<td>33</td>
</tr>
<tr>
<td>Keimer, B.</td>
<td>63</td>
</tr>
<tr>
<td>Keller, L.</td>
<td>87</td>
</tr>
<tr>
<td>Keller, T.</td>
<td>47</td>
</tr>
<tr>
<td>Kempa, M.</td>
<td>51, 99, 111</td>
</tr>
<tr>
<td>Kenzelmann, M.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Kézsmárki, I.</td>
<td>21, 23, 123, 129</td>
</tr>
<tr>
<td>Kimpton, J.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Klauada, H.</td>
<td>69</td>
</tr>
<tr>
<td>Kocsis, V.</td>
<td>123</td>
</tr>
<tr>
<td>Köhler, J.</td>
<td>96</td>
</tr>
<tr>
<td>Kolesnikov, A.</td>
<td>125</td>
</tr>
<tr>
<td>Körmann, F.</td>
<td>49</td>
</tr>
<tr>
<td>Koza, M. M.</td>
<td>43</td>
</tr>
<tr>
<td>Krannich, S.</td>
<td>47</td>
</tr>
<tr>
<td>Krawczyk, J.</td>
<td>15</td>
</tr>
<tr>
<td>Kremer, R.</td>
<td>96</td>
</tr>
<tr>
<td>Krüger, J.</td>
<td>19</td>
</tr>
<tr>
<td>Kulda, J.</td>
<td>51, 99</td>
</tr>
<tr>
<td>Kumar, C. M. N.</td>
<td>91</td>
</tr>
<tr>
<td>Kumzerov, Y.</td>
<td>125</td>
</tr>
<tr>
<td>Kuschewski, F.</td>
<td>33</td>
</tr>
<tr>
<td>Kužma, D.</td>
<td>75, 105, 121</td>
</tr>
<tr>
<td>Kyriakos, K.</td>
<td>19</td>
</tr>
<tr>
<td>Lamago, D.</td>
<td>47</td>
</tr>
<tr>
<td>Lamberti, C.</td>
<td>83</td>
</tr>
<tr>
<td>Lanceros-Méndez, S.</td>
<td>117</td>
</tr>
<tr>
<td>Larkin, T.</td>
<td>63</td>
</tr>
<tr>
<td>Lazzarin, A.</td>
<td>83</td>
</tr>
<tr>
<td>Leist, J.</td>
<td>25</td>
</tr>
<tr>
<td>Leitner, M.</td>
<td>41, 69</td>
</tr>
<tr>
<td>Leofanti, G.</td>
<td>83</td>
</tr>
<tr>
<td>Le Tacon, M.</td>
<td>57</td>
</tr>
<tr>
<td>Lhotel, E.</td>
<td>31</td>
</tr>
<tr>
<td>Łodzia, Z.</td>
<td>37</td>
</tr>
<tr>
<td>Lohstroh, W.</td>
<td>19</td>
</tr>
<tr>
<td>Loidl, A.</td>
<td>21, 23</td>
</tr>
<tr>
<td>Lokshin, K.</td>
<td>125</td>
</tr>
<tr>
<td>Lukasiewicz, T.</td>
<td>99</td>
</tr>
<tr>
<td>Lunkenheimer, P.</td>
<td>23</td>
</tr>
<tr>
<td>Maccarini, M.</td>
<td>43</td>
</tr>
<tr>
<td>Maczka, M.</td>
<td>109</td>
</tr>
<tr>
<td>Maignan, A.</td>
<td>67</td>
</tr>
<tr>
<td>Majka, M.</td>
<td>75, 105, 121</td>
</tr>
<tr>
<td>Major, M.</td>
<td>35</td>
</tr>
<tr>
<td>Martin, C.</td>
<td>67</td>
</tr>
<tr>
<td>Massalska-Arodż, M.</td>
<td>15</td>
</tr>
<tr>
<td>McIntyre, G. J.</td>
<td>97, 107</td>
</tr>
<tr>
<td>Meyer, A.</td>
<td>39</td>
</tr>
<tr>
<td>Michel, K. H.</td>
<td>79</td>
</tr>
<tr>
<td>Mignot, J-M.</td>
<td>47</td>
</tr>
<tr>
<td>Mihalik, M.</td>
<td>29</td>
</tr>
<tr>
<td>Milde, P.</td>
<td>21, 33</td>
</tr>
<tr>
<td>Mirebeau, I.</td>
<td>71, 119</td>
</tr>
<tr>
<td>Miret-Artés, S.</td>
<td>43</td>
</tr>
<tr>
<td>Mohczuki, M.</td>
<td>21</td>
</tr>
<tr>
<td>Mota, D. A.</td>
<td>29</td>
</tr>
<tr>
<td>Müller-Buschbaum, P.</td>
<td>19</td>
</tr>
<tr>
<td>Müller, U.</td>
<td>19</td>
</tr>
<tr>
<td>Murawski, J.</td>
<td>33</td>
</tr>
<tr>
<td>Murshed, M.</td>
<td>113</td>
</tr>
<tr>
<td>Muševič, I.</td>
<td>17</td>
</tr>
<tr>
<td>Mutka, H.</td>
<td>71, 119</td>
</tr>
</tbody>
</table>
Index

N
Nagel, U. 123
Narayanan, N. 97, 107
Neibecker, P. 69
Neuber, E. 33
Neugebauer, J. 49, 69
Nuzhnyy, D. 127
Nzuhnyy, D. 89

O
Ollivier, J. 71, 119
Ondrejkovič, P. 51, 99, 111

P
Papadakis, C. 19
Park, J. 59
Parlinski, K. 91
Pasciak, M. 51, 111
Passos, D. J. 29
Paul, A. 77
Pellegrini, R. 83
Petit, S. 27, 67, 71, 119
Petralanda, U. 131
Petry, W. 19, 69
Peltzeit, J. 89, 127
Pförr, F. 36
Philipp, M. 19
Pimenov, A. 93
Piovano, A. 83
Pomjakushina, E. 97, 107
Pöppl, A. 109
Pröpper, D. 63

Q
Queirós, E. 29

R
Reuvekamp, P. 95
Reynolds, N. 97, 107
Robert, J. 71, 119
Roessli, B. 35
Rols, S. 67, 91
Roöm, T. 123
Ross, M. 41
Rost, A. 63
Rotundu, C. 61
Rovillain, P. 97, 107
Roy, P. 27
Rozwadowski, T. 15
Rüegg, C. 87

S
Sacuto, A. 55
Samulionis, V. 117
Schneidewind, A. 137
Schranz, W. 73
Sepiol, B. 41
Sidis, Y. 47
Silbin, M. 117
Šimėnas, M. 109
Simeoni, G. 39
Simonet, V. 27
Sobieszczyk, P. 75, 105, 121
Sobolev, O. 113
Stana, M. 41
Stasinopoulos, I. 23
Steffens, P. 47
Stejskal, J. 127
Sternberg, A. 101
Stuhr, U. 35
Svirskas, S. 101, 117
Szaller, D. 129

T
Taguchi, Y. 123
Takagi, H. 63
Takayama, T. 63
Tavares, P. 29
Telling, M. T. F. 43
Tokunaga, Y. 123
Tokura, Y. 123
Trchová, M. 127
Tröster, A. 81
Tsurkan, T. 23
Tsurkan, V. 21

U
Ulrich, C. 97, 107

V
Vakhrušev, S. 125
Vilarinho Silva, R. 29
Von Löhneysen, H. 47

W
Wang, Z. 23
Wasik, M. 103
Wdowik, U. 103
Wdowik, U. D. 91
Weber, F. 47
Weber, T. 133
Wehinger, B. 61, 87, 115
Welberry, T. R. 51
White, J. 21

Y
Yang, F. 39
Yang, J. J. 129
Yaresko, A. 63
Yethiraj, M. 97, 107

Z
Zbiri, M. 43
Zentková, M. 29
Ziegler, F. 25, 113
Zieliński, P. 75, 105, 121
<table>
<thead>
<tr>
<th>List of participants</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ALMEIDA Abílio</strong></td>
</tr>
<tr>
<td><strong>ARAII Masatoshi</strong></td>
</tr>
<tr>
<td><strong>BANYS Juras</strong></td>
</tr>
<tr>
<td><strong>BÖNI Peter</strong></td>
</tr>
<tr>
<td><strong>BORIS Alexander</strong></td>
</tr>
<tr>
<td><strong>BUJAKIEWICZ-KORONSKA Renata</strong></td>
</tr>
<tr>
<td><strong>BUSSMANN-HOLDER Annette</strong></td>
</tr>
<tr>
<td><strong>ČERMÁK Petr</strong></td>
</tr>
<tr>
<td><strong>CHANG Johann</strong></td>
</tr>
<tr>
<td><strong>CHUMAKOV Aleksandr</strong></td>
</tr>
<tr>
<td><strong>DAMAY Françoise</strong></td>
</tr>
<tr>
<td><strong>DE BRION Sophie</strong></td>
</tr>
<tr>
<td><strong>ECKOLD Götz</strong></td>
</tr>
<tr>
<td><strong>ENG Lukas</strong></td>
</tr>
<tr>
<td><strong>ETXEBARRIA Inigo</strong></td>
</tr>
<tr>
<td><strong>EVENSON Zach</strong></td>
</tr>
<tr>
<td><strong>FORREST Thomas</strong></td>
</tr>
<tr>
<td><strong>FOUQUET Peter</strong></td>
</tr>
<tr>
<td><strong>FULTZ Brent</strong></td>
</tr>
<tr>
<td><strong>GIBHARDT Holger</strong></td>
</tr>
<tr>
<td><strong>GRAHAM Paul</strong></td>
</tr>
<tr>
<td><strong>HACKL Rudolf</strong></td>
</tr>
<tr>
<td><strong>HLINKA Jiri</strong></td>
</tr>
<tr>
<td><strong>IVANOV Alexandre</strong></td>
</tr>
<tr>
<td><strong>IVANOVA Oxana</strong></td>
</tr>
<tr>
<td><strong>JAHN Sandro</strong></td>
</tr>
<tr>
<td><strong>JOCHYM Pawel T.</strong></td>
</tr>
<tr>
<td><strong>KAMBA Stanislav</strong></td>
</tr>
<tr>
<td><strong>KELLER Thomas</strong></td>
</tr>
<tr>
<td><strong>KEMPA Martin</strong></td>
</tr>
<tr>
<td><strong>KÉZSMÁRTI István</strong></td>
</tr>
<tr>
<td><strong>KOCSIS Vilmos</strong></td>
</tr>
<tr>
<td><strong>KRAWCZYK Jan</strong></td>
</tr>
<tr>
<td><strong>KULDA Jiri</strong></td>
</tr>
<tr>
<td><strong>KUŹMA Dominika</strong></td>
</tr>
<tr>
<td>Name</td>
</tr>
<tr>
<td>------</td>
</tr>
<tr>
<td>LE TACON Mathieu</td>
</tr>
<tr>
<td>LEITNER Michael</td>
</tr>
<tr>
<td>L'HOTEL Elsa</td>
</tr>
<tr>
<td>ŁODZIANA Zbigniew</td>
</tr>
<tr>
<td>LOIDL Alois</td>
</tr>
<tr>
<td>MAJKA Marcin</td>
</tr>
<tr>
<td>MEDALA Magdalena</td>
</tr>
<tr>
<td>MICHEL Karl H.</td>
</tr>
<tr>
<td>MOREIRA Joaquim Agostinho</td>
</tr>
<tr>
<td>MUŠEVIĆ Igor</td>
</tr>
<tr>
<td>NEIBECKER Pascal</td>
</tr>
<tr>
<td>NEMKOVSKY Kirill</td>
</tr>
<tr>
<td>NEUGBAUER Jörg</td>
</tr>
<tr>
<td>NEUHAUS Jürgen</td>
</tr>
<tr>
<td>ONDREJKOVIČ Petr</td>
</tr>
<tr>
<td>PARK Jitae</td>
</tr>
<tr>
<td>PASCIAK Marek</td>
</tr>
<tr>
<td>PAUL Amitesh</td>
</tr>
<tr>
<td>PETIT SYLVAIN</td>
</tr>
<tr>
<td>PETRY Winfried</td>
</tr>
<tr>
<td>PETZELT Jan</td>
</tr>
<tr>
<td>PFORR Florian</td>
</tr>
<tr>
<td>PHILIPP Martine</td>
</tr>
<tr>
<td>PIMENOV Andrei</td>
</tr>
<tr>
<td>PIOVANO Andrea</td>
</tr>
<tr>
<td>SACUTO Alain</td>
</tr>
<tr>
<td>SAMULIONIS Vytautas</td>
</tr>
<tr>
<td>SCHNEIDEWIND Astrid</td>
</tr>
<tr>
<td>SCHRANZ Wilfried</td>
</tr>
<tr>
<td>SOBIESZCZYK Paweł</td>
</tr>
<tr>
<td>SPEZIALE Sergio</td>
</tr>
<tr>
<td>STANA Markus</td>
</tr>
<tr>
<td>SU Yixi</td>
</tr>
<tr>
<td>SZALLER David</td>
</tr>
<tr>
<td>Name</td>
</tr>
<tr>
<td>-----------------------</td>
</tr>
<tr>
<td>TRÖSTER Andreas</td>
</tr>
<tr>
<td>ULRICH Clemens</td>
</tr>
<tr>
<td>VILARINHO SILVA Rui</td>
</tr>
<tr>
<td>WDOWIK Urszula D.</td>
</tr>
<tr>
<td>WEBER Tobias</td>
</tr>
<tr>
<td>WEBER Frank</td>
</tr>
<tr>
<td>WEHINGER Bjoern</td>
</tr>
<tr>
<td>WUTTKE Joachim</td>
</tr>
<tr>
<td>ZIEGLER Fabian</td>
</tr>
<tr>
<td>ZIELINSKI Piotr</td>
</tr>
</tbody>
</table>

**Imprint**

**Contact**

Technische Universität München  
Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)  
Heinz Maier-Leibnitz Zentrum (MLZ)  
Lichtenbergstraße 1  
D-85748 Garching  

dyproso2015@frm2.tum.de

**Editors**

Elisabeth Jörg-Müller, FRM II / MLZ  
Michael Leitner, MLZ / TUM  
Pascal Neibecker, FRM II / MLZ  
Jürgen Neuhaus, FRM II / MLZ  
Winfried Petry, FRM II / MLZ

**Design, Layout and Typesetting**

Ramona Bucher, JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

**Picture credits**

Kardinal-Döpfner-Haus  
Cover top, Page 8  
W. Schürmann/ TUM  
Cover below
At the Heart of Cathedral City
A walking tour of Freising’s Old Quarter and Weihenstephan Hill

Freising’s History
Cathedral Hill, from which the two Romanesque towers of Freising Cathedral ascend, was the spiritual and cultural heart of Old Bavaria for many centuries and the seat of a host of famous scholars. Historian and bishop Otto of Freising was a successor of St. Corbinian. The Freising prince-bishops expanded their royal seat and Cathedral Hill into a seat of government saturated with magnificent architecture and works of art. Today Freising is a university city, as well as an important economic centre for reasons including its proximity to Munich Airport. A vibrant cultural scene and the universal Old Bavarian spirit of hospitality in the city and its restaurants and inns help to make Freising a popular meeting-point for connoisseurs and pleasure-seekers.

Marienplatz with Marienbild

The Baroque Column of Mary (1674) is the centre of Marienplatz square, the bustling heart of the city and starting-point for all walks through the Old Quarter.

Town Hall
The early 20th-century historicist building perfectly complements the architectural ensemble around Marienplatz.

St. Georg
An impressive Baroque tower (1661/1669) soars over the Late Gothic nave church. Picturesque winding lanes lined with historical houses lie in its shade.

Zierer-Haus
The former townhouse (Built 1720), with its magnificent neoclassic façade, is testimony to the wealth of the bourgeoisie in the 18th-century city. Today it houses the City of Freising registry office.

Asamkirche (former Prince-Bishop’s Lyceum)
The “Asam Building” was built in 1697. The hall was decorated with Baroque frescoes by Oraz Asam, father of the famous brothers Cosmas Damian Asam and Egid Quirin Asam. It is used today for theatre performances, concerts and conferences. The building also houses the City Museum, with impressive exhibitions tracing the turbulent history of the prince-bishops’ seat and later Bavarian provincial city, as well as the City of Freising Tourist Information Office.

Bürgerturn Tower
A mile of the historical city fortifications.

Cathedral Hill
Cathedral Hill is a repository for art and artworks spanning the epochs and collected by the prince-bishops and others, towering over the secular city. It was a haven of scholarship for centuries.

Marienbild Cathedral
One of Bavaria’s major sights, this Romanesque cathedral with hall crypt and beasts’ pillar was redesigned in the Baroque style by the Asam brothers in the 18th century, when many works of art were introduced.

Bishop Otto of Freising
The monument by Caspar von Zumbusch, commemorating the most important philosopher of history of the Middle Ages, was erected on the site of the earlier Moor’s Fountain in 1857.

Residence
The former prince-bishops’ residence today houses the Education Centre of the Archdiocese of Munich–Freising.

Diocesan Museum
The internationally famous art collection contains precious religious art from the Alpine region throughout all epochs up to contemporary times.

Neustift
The church of the former Premonstratensian Abbey of Neustift is ornamented with ceiling frescoes by Johann Baptist Zimmermann and altar figures by Ignaz Günther.

Weihenstephan St. Corbinian’s Spring and the ruined Benedictine monastery are among the relics bearing witness to Weihenstephan’s spiritual past. Today the Weihenstephan Hill campus contains the modern buildings of the TU Munich–Weihenstephan, Weihenstephan-Triesdorf College and numerous institutes, colleges and research centres.

Weihenstephan Brewery
The “oldest brewery in the world”, located in the former Weihenstephan monastery, is owned by the Free State of Bavaria.

Zentrale Touristinformationen
Central Tourist Information Office
Officina del turismo azienda
Emplacement de l’information touristique

Parkplatz
Car park – Parking – Parkeggio

Parksauß
Multi-storey car park
Parking covered – Parking à couverture

Busparkplatz
Coach park – Parkeggio per bus

Polizei
Police – Police – Polizia

Öffentliche Toilette
(behindertengerecht)
Public toilets (suitable for disabled)
Toîttes publiques (access PPR usable)
Servicio público (accesible para discapacitados)

Krankenhaus
Hospital – Hospital – Ospedale

Post
Post office – Bureau de Poste
Office Postale

Kirche
Church – Chiesa

Denkmal
Monument – Monumento

Monumento

Monument

Monumento
<table>
<thead>
<tr>
<th>Sunday, 13 September</th>
<th>Monday, 14 September</th>
<th>Tuesday, 15 September</th>
<th>Wednesday, 16 September</th>
<th>Thursday, 17 September</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00</td>
<td>08:30</td>
<td>08:30</td>
<td>08:30</td>
<td>08:30</td>
</tr>
<tr>
<td>Welcome</td>
<td>Z. Lodziana</td>
<td>A. Sacuto</td>
<td>S. Jahn</td>
<td>S. Jahn</td>
</tr>
<tr>
<td>09:10</td>
<td>09:10</td>
<td>09:10</td>
<td>09:10</td>
<td>09:10</td>
</tr>
<tr>
<td>A. Chumakov</td>
<td>Z. Evenson</td>
<td>M. Le Tacon</td>
<td>B. Wehinger</td>
<td>B. Wehinger</td>
</tr>
<tr>
<td>J. Krawczyk</td>
<td>09:35</td>
<td>09:50</td>
<td>09:35</td>
<td>09:35</td>
</tr>
<tr>
<td>10:15</td>
<td>M. Stana</td>
<td>J. Park</td>
<td>S. Kamba</td>
<td>S. Kamba</td>
</tr>
<tr>
<td>M. Philipp</td>
<td>10:00</td>
<td>10:15</td>
<td>10:15</td>
<td>10:15</td>
</tr>
<tr>
<td>10:40</td>
<td>10:55</td>
<td>10:10</td>
<td>10:10</td>
<td>10:10</td>
</tr>
<tr>
<td>Coffee break</td>
<td>B. Fultz</td>
<td>J. Chang</td>
<td>A. Pimenov</td>
<td>A. Pimenov</td>
</tr>
<tr>
<td>11:10</td>
<td>11:35</td>
<td>11:50</td>
<td>11:50</td>
<td>11:50</td>
</tr>
<tr>
<td>I. Musevic</td>
<td>F. Weber</td>
<td>A. Boris</td>
<td>A. Bussmann-Holder</td>
<td>A. Bussmann-Holder</td>
</tr>
<tr>
<td>11:50</td>
<td></td>
<td></td>
<td>F. Ziegler</td>
<td></td>
</tr>
<tr>
<td>F. Ziegler</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12:15 Lunch</td>
<td>12:00 Lunch</td>
<td>12:15 Lunch</td>
<td>12:15 Lunch</td>
<td>12:15 Lunch</td>
</tr>
<tr>
<td>I. Kezmarksi</td>
<td>J. Neugebauer</td>
<td>F. Damay</td>
<td>C. Ulrich</td>
<td>C. Ulrich</td>
</tr>
<tr>
<td>A. Loidl</td>
<td>M. Pasciak</td>
<td>S. Petit</td>
<td>P. Ondrejkovic</td>
<td>P. Ondrejkovic</td>
</tr>
<tr>
<td>14:35</td>
<td></td>
<td>14:20</td>
<td>14:20</td>
<td>14:20</td>
</tr>
<tr>
<td>S. de Brion</td>
<td></td>
<td>P. Neibecker</td>
<td>J. Banys</td>
<td>J. Banys</td>
</tr>
<tr>
<td>14:35</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Hlinka</td>
<td></td>
<td></td>
<td>End of the conference</td>
<td>End of the conference</td>
</tr>
<tr>
<td>15:00</td>
<td>15:00</td>
<td>14:45</td>
<td>and Coffee</td>
<td>and Coffee</td>
</tr>
<tr>
<td>Coffee break</td>
<td>15:00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15:30</td>
<td>15:30</td>
<td>15:15</td>
<td>15:15</td>
<td>15:15</td>
</tr>
<tr>
<td>R. Vilarinho Silva</td>
<td>Guided tours</td>
<td>W. Schranz</td>
<td>M. Majka</td>
<td>M. Majka</td>
</tr>
<tr>
<td>15:30</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17:00 Registration</td>
<td>15:55</td>
<td>18:00</td>
<td>16:05</td>
<td>16:05</td>
</tr>
<tr>
<td>E. Lhotel</td>
<td>Dinner or snack</td>
<td>A. Paul</td>
<td>A. Paul</td>
<td>A. Paul</td>
</tr>
<tr>
<td>16:35</td>
<td>at FRM II</td>
<td>16:45</td>
<td>16:45</td>
<td>16:45</td>
</tr>
<tr>
<td>L. Eng</td>
<td></td>
<td>K.H. Michel</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17:15</td>
<td></td>
<td>A. Tröster</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F. Pforr</td>
<td></td>
<td>17:35</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18:00 Dinner</td>
<td>18:00</td>
<td>17:00</td>
<td>17:00</td>
<td>17:00</td>
</tr>
<tr>
<td>19:00 Welcome</td>
<td>19:00</td>
<td>19:00</td>
<td>19:30</td>
<td>19:30</td>
</tr>
<tr>
<td>Reception</td>
<td>Poster session</td>
<td>Advisory Board</td>
<td>Conference Dinner</td>
<td>Conference Dinner</td>
</tr>
<tr>
<td>19:00</td>
<td></td>
<td>Meeting</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19:30</td>
<td></td>
<td>19:30</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Amorphous and Soft Matter**
- **Multiferroics and Ferroelectrics**
- **Electrons and spins**
- **Diffusive dynamics**
- **Phonons and Magnons**
- **Theoretical and Experimental Methods**
- **Excitations of Strongly Correlated Electron Systems**
- **Two-dimensional Systems**
- **Materials under High Pressure**
- **Poster Session**