39th International Symposium on Dynamical Properties of Solids

Abstract Book

Dresden, 25 – 29 September 2023

TECHNISCHE UNIVERSITÄT DRESDEN

ACKNOWLEDGEMENTS – SPONSORS

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ACKNOWLEDGEMENTS – PARTNERS

We cordially thank our COOPERATION PARTNERS:

the → **Technische Universität Dresden**,

the → **Leibniz Institute of Solid State and Materials Research (IFW) Dresden**,

and the → **Helmholtz-Zentrum Dresden-Rossendorf**,

all being connected within the → **DRESDEN concept** network.

Contents

Welcome

The 39th International Symposium on Dynamical Properties of Solids – DyProSo-2023 – will take place between September 25 – 29, 2023 in Dresden, Germany.

DyProSo is an international biannual research meeting devoted to the research on functional properties of condensed matter that result from elementary excitations, molecular motions, transport processes, and other dynamic phenomena occurring in many body systems. Discussions on experimental evidences and investigations, as well as theoretical models and predictions are of particular relevance at DyProSo-2023.

A special purpose of this DyProSo Symposium is to trigger the scientific dialogue between young and experienced researchers exploring the working in the field of dynamics of materials.

Especially, the following topics will be addressed:

- Dynamic properties of matter.
- Phonons, plasmons, magnons, polaritons, electromagnons, spins.
- (Multi)ferroic materials.
- Strongly correlated electron systems.
- Low-dimensional structures.
- Disordered, amorphous and soft matter.
- Materials under extreme conditions.
- Frontiers of experimental and theoretical methods.

Visit our website for **late-breaking information** before and during the symposium:

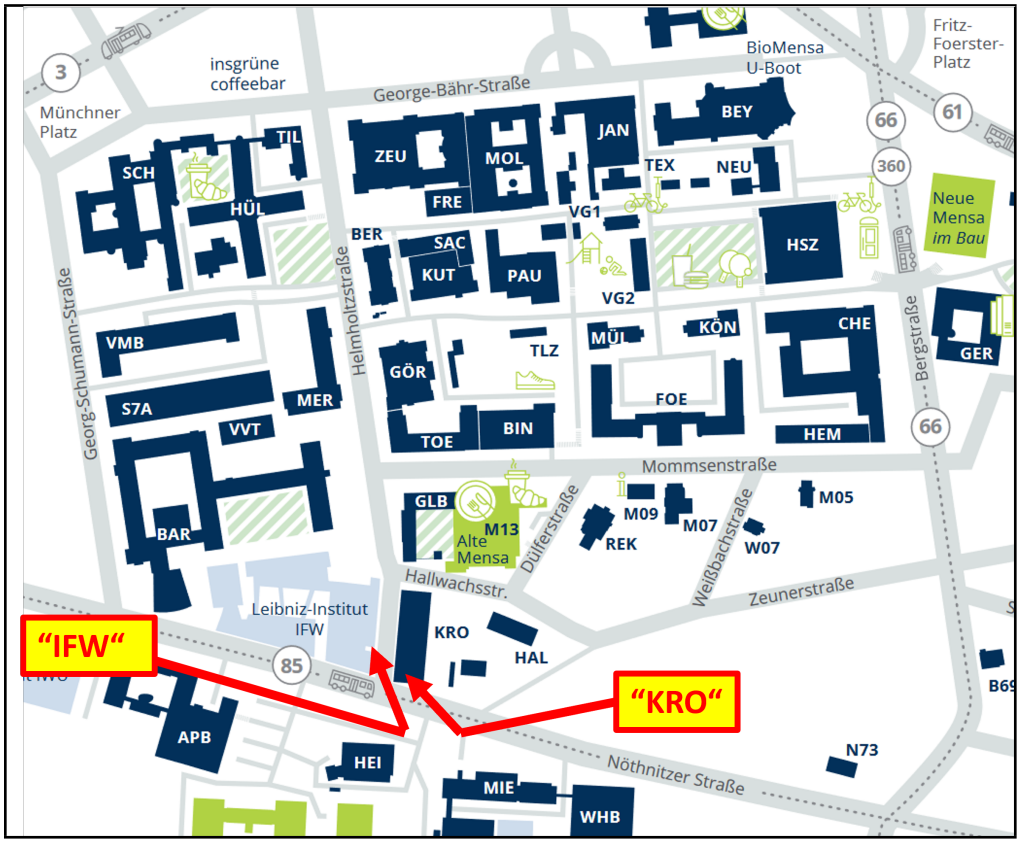
https://dyproso-2023.com/

Local organization: **Prof. Lukas M. Eng**
Institute of Applied Physics
Technische Universität Dresden

Venue

The DyProSo-2023 takes place in two neighbouring buildings – in the Hermann-Krone-Bau (→**"KRO"**) and the lecture hall of the Leibniz Institute of Solid State and Materials Research Dresden (→**"IFW"**) – both located within the → **main campus of TU Dresden**, which can be reached easily by public transport (→ **use journey planner**), with the following nearest bus-/tram-stops:

Helmholtzstraße (bus line 85, almost in front of the KRO/IFW entrances),
Mommsenstraße (bus line 66, 5-min walk),
Technische Universität (bus lines 61 or 66, 10-min walk),
Nürnberger Platz (tram lines 3 and 8, 10-min walk), or
Münchner Platz (tram line 3, 5-min walk).



- On September, 25th, **registration and welcome reception** will start at 04:00 p.m. at TU Dresden's Institute of Applied Physics (IAP) located in **Hermann-Krone-Bau, 1st floor, and at the roof terrace, 2nd floor**.

  → **Hermann-Krone-Bau (KRO), Nöthnitzer Straße 61, 01187 Dresden [Google Maps]**

  → **Hermann-Krone-Bau [Campus Navigator]**

- The **conference sessions** from September 26th–28th are held in the **lecture hall of the Leibniz Institute for Solid State and Materials Research Dresden** (IFW Dresden).

  → **IFW Dresden, Helmholtzstraße 20, 01069 Dresden [Google Maps]**

- The **conference dinner** on September, 27th will take place at → **Café Vis-á-Vis** on Brühl's Terrace (Brühlsche Terrasse) in Dresden's historical old town.

- The full-time **excursion to Helmholtz-Center Dresden-Rossendorf (→ HZDR)** on Friday, September 29th, comprises visits of two large-scale experimental facilities: the "Free-Electron Laser" Laboratory (FELBE) and the "High-Magnetic-Field" Laboratory (HLD). For the detailed schedule, refer to the conference website's → **excursion page**.

Schedule – Overview

Monday, September, 25th		
04:00 – 07:00 p.m.	Registration & Welcome Reception	Hermann-Krone-Bau: 1st Floor / Roof Terrace
Tuesday, September, 26th		
08:00 – 08:45 a.m.	Registration	Foyer of IFW Lecture Hall
08:45 – 09:00 a.m.	**Welcome** (15 min)	IFW Lecture Hall
09:00 – 10:00 a.m.	**Keynote Talk I** (60 min)	IFW Lecture Hall
10:00 – 10:30 a.m.	Coffee Break (30 min)	
10:30 – 12:25 a.m.	**Session 1** (115 min)	IFW Lecture Hall
12:30 – 01:30 p.m.	Lunch Break (60 min)	
01:30 – 03:00 p.m.	**Session 2 (Poster Session)** (90 min)	Foyer of IFW Lecture Hall
03:00 – 03:30 p.m.	Coffee Break (30 min)	
03:30 – 05:50 p.m.	**Session 3** (140 min)	IFW Lecture Hall
06:30 – 07:30 p.m.	*DyProSo-Advisory-Board Meeting*	Hermann-Krone-Bau, Room 1.11 A
Wednesday, September, 27th		
09:00 – 10:00 a.m.	**Keynote Talk II** (60 min)	IFW Lecture Hall
10:00 – 10:30 a.m.	Coffee Break (30 min)	
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01:30 – 03:30 p.m.	**Excursion I** (120 min)	SLUB/KRO[1]
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10:30 – 12:25 a.m.	**Session 6** (115 min)	IFW Lecture Hall
12:30 – 01:30 p.m.	Lunch Break (60 min)	
01:30 – 03:00 p.m.	**Session 7** (90 min)	IFW Lecture Hall
03:00 – 03:30 p.m.	Coffee Break (30 min)	
03:30 – 05:20 p.m.	**Session 8** (110 min)	IFW Lecture Hall
05:20 – 05:30 p.m.	**Closing** (10 min)	
Friday, September, 29th: Excursion II – Helmholtz-Zentrum Dresden-Rossendorf (HZDR)		
08:00 – 09:00 a.m.	Bus transfer from Dresden	Meeting point: Hermann-Krone-Bau
09:00 – 10:00 a.m.	**Welcome / Introduction to HZDR**	
10:00 – 12:00 p.m.	**Guided tours of HLD[2] and ELBE[3]**	
12:30 – p.m.	Lunch	"Lodge at the lake" (after a 20-min. walk)
– 04:00 p.m.	Arrival back in Dresden (via Bus)	Final destination: Hermann-Krone-Bau

[1] Visits of the treasure chamber of the University Library (SLUB) and the Hermann Krone Collection.
[2] High Magnetic Field Laboratory (HLD)
[3] Center for High-Power Radiation Sources (ELBE)

Scientific Program

Tuesday, September, 26th

08:00–08:45		Registration	

Welcome · 08:45 a.m. – 09:00 a.m. (15 min)

08:45–09:00	Welcome by	*Prof. Lukas M. Eng*, Chair of the DyProSo-2023	

Keynote Talk I · 09:00 a.m. – 10:00 a.m. (60 min) · Chair: Samuel Seddon

09:00–10:00	J. Wosnitza	Materials Research in Very High Magnetic Fields	1

Session 1 (ME – Magnetolectrics) · 10:30 a.m. – 12:25 p.m. (115 min) · Chair: Dalibor Repček

10:30–11:10	W. Blackmore	Slow magnetic reversal in a highly axial paramagnetic dysprosium compound	2
11:10–11:35	M. Brioschi	Investigation of magnetoelastic coupling in Fe(10 nm)/Py(10 nm) nanowire array	3
11:35–12:00	D. Kuźma	Switching Mechanisms in 1D System of Elongated Shaped Thin Magnetic Particles	4
12:00–12:25	S. Kamba	Magnetoelectric properties of Fe^{3+} substituted multiferroic $TbMnO_3$	5

Session 2 (Posters) · 01:30 p.m. – 03:00 p.m. (90 min) · !!! Posters can stay for 3 days !!!

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P 02	A. Devillez	Investigating the magnetic properties of $BaCo_2(AsO_4)_2$: Magnetisation steps and Hamiltonian simulation	7
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Tuesday, September, 26th (continued)

Session 3 (FE I – Ferroelectrics I) ·

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Wednesday, September, 27th

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05:20–05:30		Closing remarks by L. M. Eng

List of presenting authors

Abstracts

Colour code:

- **Keynote Talks**
- **Invited Talks**
- **Contributed Talks**
- **Posters**

Tuesday, 26$^{\text{th}}$ Sep 2023

Materials Research in Very High Magnetic Fields

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High magnetic fields are one of the most powerful tools available to scientists for the study, modification, and control of the state of matter. The application of magnetic fields, therefore, has become a commonly used instrument in materials-science research and the demand for the highest possible magnetic-field strengths increases continuously. The High Magnetic Field Laboratory Dresden (Hochfeld-Magnetlabor Dresden, HLD) at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) makes available pulsed magnetic fields up to the 90 T range, on a 10 ms timescale, for in-house and external users. The HLD is part of the European Magnetic Field Laboratory (EMFL) with further sites in Grenoble and Nijmegen, for static fields, and in Toulouse for pulsed fields. In the pulsed magnets, a variety of experimental methods are available enabling to measure, for example, electrical transport, magnetization, dilatometry, ultrasound, ESR, and even NMR with very high resolution. As a unique feature, a free-electron-laser facility next door allows high-brilliance radiation to be fed into the pulsed-field cells of the HLD, thus making possible high-field magneto-optical experiments in the range from 5 to 250 µm. In-house research of the HLD focuses on electronic properties of strongly correlated and topological materials at high magnetic fields. This includes the investigation of novel frustrated magnetic materials and the determination of Fermi surfaces of topological and correlated metals by means of measurements of magnetic quantum oscillations. We further investigate unconventional high-magnetic-field states of novel superconductors, but, beyond that, even field-induced plasma waves in liquid metals. Here, I will present a brief overview on the experimental infrastructure and discuss some highlights of the in-house research at the Dresden High Magnetic Field Laboratory.

Slow magnetic reversal in a highly axial paramagnetic dysprosium compound

William J. A. Blackmore[1], Gemma K. Gransbury[1], Andrea Mattioni[1], Sophie C. Corner[1], Peter Evans[1], Jon G. C. Kragskow[1,2], Daniel Reta[1,3], David P. Mills[1], and Nicholas F. Chilton[1]

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[3] Kimika Fakultatea, Euskal Herriko Unibertsitatea, UPV/EHU, Donostia International Physics Center (DIPC), IKERBASQUE, Basque Foundation for Science, Donostia, Euskadi, Bilbao, Spain

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Single molecule magnets are highly axial paramagnetic compounds with a large energy barrier to magnetic reversal. These slowly magnetically relaxing systems show great potential to be used in classical data storage and participate in the second quantum revolution [1]. However, challenges remain in chemically controlling the magnetic reversal. This is partly due to experimental limitations and a lack of consistency when characterising the slowest relaxing materials ($\tau \gtrsim 10^4$ s) with wide underlying distributions [2].

We have developed guidelines on the experimental design, data fitting, and analysis required to accurately interpret magnetisation decay measurements. Using this new protocol, we performed magnetisation decays and sweeps on pure and solution samples of the high-performing single-molecule magnet $[Dy(Cp^{ttt})_2][B(C_6F_5)_4]$ ($Cp^{ttt} = C_5H_2{}^tBu_3$-1,2,4; $^tBu = C(CH_3)_3$), to probe how different phonon environments affects magnetic reversal and the quantum tunnelling gap of the ground-state avoided crossing at zero-field [3].

[1] Matteo Atzori and Roberta Sessoli, *The Second Quantum Revolution: Role and Challenges of Molecular Chemistry*, Journal of the American Chemical Society **141**, 11339–11352 (2019).

[2] William J. A. Blackmore, Gemma K. Gransbury, Peter Evans, Jon G. C. Kragskow, David P. Mills and Nicholas F. Chilton, *Characterisation of magnetic relaxation on extremely long timescales*, Physical Chemistry Chemical Physics **25**, 16735–16744 (2023).

[3] William J. A. Blackmore, Andrea Mattioni, Sophie C. Corner, Peter Evans, Gemma K. Gransbury, David P. Mills, and Nicholas F. Chilton, *Measurement of the Quantum Tunneling Gap in a Dysprosocenium Single-Molecule Magnet*, Journal of Physical Chemistry Letters **14**, 2193–2200 (2023).

Investigation of magnetoelastic coupling in Fe(10 nm)/Py(10 nm) nanowire array

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Nowadays, the control of coherent collective spin excitations in magnetically ordered materials at the nanoscale is one of the most promising concepts for the development of novel and energy-efficient information technologies. In particular, a powerful approach to manipulate spin waves is to exploit the hybridization of magnons with phonons [1, 2, 3].

We report on the hybrid magneto-mechanical properties of a 1D magnonic crystal composed of Fe(10 nm)/ Py(10 nm) bilayered nanowires [4]. An infrared laser pulse triggers both acoustic and spin waves, and the system behaves as a magneto-mechanical cavity when an external magnetic field is properly tuned. We investigate the magneto-elastic coupling by analysis of time-resolved reflectivity and time-resolved MOKE. We observe two non-dispersive magnetoelastic (MEC) modes and a purely magnetic one. In particular, we focus on the dispersion of the latter and its crossing with the MEC modes, which exhibits features depending on the sample orientation with respect to the external magnetic field. Results are in good qualitative and quantitative agreement with Brillouin light scattering measurements and micromagnetic simulations, providing interesting insight into phonon-magnon coupling in magnonic crystals.

Acknowledgements Research at IOM-CNR has been funded by the European Union - NFFA-Europe-Pilot under H2020 grant agreement n. 101007417 and NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem grant ECS00000041 - VITALITY. G. Gubbiotti and G. Panaccione acknowledge Università degli Studi di Perugia, CNR and MUR for support within the project Vitality.

[1] H. Hayashi and K. Ando, *Spin Pumping Driven by Magnon Polarons*, Physical Review Letters **121**, 237202 (2018).

[2] C. Berk, M. Jaris, et al., *Strongly coupled magnon–phonon dynamics in a single nanomagnet*, Nature Communications **19**, 2652 (2019).

[3] F. Godejohann, A. V. Scherbak, et al., *Magnon polaron formed by selectively coupled coherent magnon and phonon modes of a surface patterned ferromagnet*, Physical Review B **102**, 144438 (2020).

[4] G. Gubbiotti, S. Tacchi, et al., *Collective spin excitations in bicomponent magnonic crystals consisting of bilayer permalloy/Fe nanowires*, Physical Review B **93**, 184411 (2016).

Switching Mechanisms in 1D System of Elongated Shaped Thin Magnetic Particles

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Well-structured sequences of stable magnets are of interest for the development of memory storage devices. Our research focused on investigating magnetization switching in linearly arranged particles with different shapes and interparticle distances under variations of a perpendicular external magnetic field. We employed various approximations suitable for macrospins, ranging from an extended Stoner-Wohlfarth model to a 1D model of magnetic threads, and extensive micromagnetic calculations that accurately represented the particle's shape [1, 2, 3, 4, 5, 6].

We observed a qualitative difference in the behaviour of infinite and finite chains. Infinite chains tend to switch the magnetization directly in a single step, while chains with a finite number of particles exhibited a sequential reversal of macrospins, resulting in several intermediate configurations with well-defined magnetizations. Some of these reversal sequences were found to be repeatable, making them promising models for multi-stage memory elements.

The numerical calculations were performed at Poznan Supercomputing and Networking Center (Grant No. 424).

[1] L. Exl, S. Bance, F. Reichel, T. Schrefl, H. P. Stimming, and N. J. Mauser, *LaBonte's method revisited: An effective steepest descent method for micromagnetic energy minimization*, Journal of Applied Physics **115**(17), 17D118 (2014).

[2] A. Vansteenkiste, J. Leliaert, M. Dvornik, M. Helsen, F. Garcia-Sanchez, and B. V. Waeyenberge, *The design and verification of MuMax3*, AIP Advances **4**(10), 107133 (2014).

[3] D. Kuźma, F. Montoncello, P. Sobieszczyk, A. Wal, L. Giovannini, and P. Zieliński, *Spin wave propagation properties across configurational antiferro/ferro-magnetic transitions*, Journal of Applied Physics **124**(22), 223902 (2018).

[4] D. Kuźma and P. Zieliński, *Finite Length Effects on Switching Mechanisms in Chains of Magnetic Particles*, Magnetochemistry **6**(4), 47 (2020).

[5] D. Kuźma, Ł. Laskowski, J. W. Kłos, and P. Zieliński, *Effects of shape on magnetization switching in systems of magnetic elongated nanoparticles*, Journal of Magnetism and Magnetic Materials **545**, 168685, doi: 10.1016/j.jmmm.2021.168685 (2022).

[6] D. Kuźma, O. Pastukh, and P. Zieliński, *Spacing Dependent Mechanisms of Remagnetization in 1D System of Elongated Diamond Shaped Thin Magnetic Particles*, Magnetochemistry **8**(9), 102 (2022).

Magnetoelectric properties of Fe^{3+} substituted multiferroic $TbMnO_3$

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Magnetoelectric multiferroics, where spontaneous long-range magnetic and dipolar order coexist, represent a very attractive class of compounds combining rich and fascinating fundamental physics with a potential for multifunctional applications. One of the most well-known multiferroics is $TbMnO_3$, exhibiting the orthorhombic *Pbnm* structure at room conditions. At $T_N = 41$ K, $TbMnO_3$ undergoes a para-antiferromagnetic phase transition with an incommensurate sinusoidal collinear ordering of the Mn^{3+} spins [1]. Below $T_c = 28$ K, a cycloid spiral spin ordering in the *bc* plane is stabilized. The cycloidal spiral antiferromagnetic phase is also ferroelectric, with the electric polarization along the *c*-axis [1]. The emergence of the ferroelectric polarization has been described in the framework of the Dzyaloshinskii-Moriya interaction between nonparallel spins. Furthermore, depending on its direction, an applied magnetic field can either suppress ferroelectricity or rotate the spin cycloidal from the *bc*- to the *ab*-plane, and thus, the electric polarization to the *a*-axis [1]. Beyond this, dynamical magnetoelectricity in $TbMnO_3$ was also identified in the form of electromagnons, i.e., magnons excitable by an electric field [2].

Rare-earth manganites are known to exhibit a strong coupling between magnetism and lattice, which can be manipulated to tailor their physical properties. In this regard, chemical substitution has been extensively used to modify properties and induce new thermodynamic phases in these compounds. Previous studies carried out in $TbMnO_3$ ceramics show that the substitution of Mn^{3+} by small amounts of the identically sized Fe^{3+} ion profoundly changes both magnetic and polar structures, altering the magnetoelectric coupling [3]. In fact, for an Fe^{3+} concentration above 5%, the multiferroic properties of the $TbMn_{1-x}Fe_xO_3$ solid solution are lost [3]. Nonetheless, as these studies were done in ceramics, anisotropic effects could not be ascertained.

In this work, the temperature and magnetic field dependence of the magnetic, dielectric and magnetoelectric properties of oriented single crystals of $TbMn_{1-x}Fe_xO_3$ with $x = 0.02$ and 0.04 were studied along all crystallographic directions [4]. It was found that, even in such low concentrations, the presence of Fe^{3+} has a striking impact in the magnetoelectric coupling. In particular, the cycloidal structure appears to be at an angle with the *c*-axis and the way the Tb^{3+} spin alignment affects the polarization depends both on Fe-concentration and applied magnetic field. The effect on the magnetic structure was studied in detail by neutron diffraction. Most changes are mainly manifest in the magnetic field dependence of the electric polarization and in the electromagnon spectra, whose temperature dependence was studied through THz time-domain spectroscopy. An overview of the main results will be presented, highlighting the contrast with previously reported studies on the unsubstituted compound.

[1] T. Kimura *et al.*, PRB **71**, 224425 (2005).

[2] Y. Takahashi *et al.*, PRB **101**, 187201 (2008).

[3] R. Vilarinho *et al.*, JMMM **439**, 167 (2017).

[4] A. Maia, R. Vilarinho *et al.*, in preparation (2023).

High-speed domain wall imaging using broadband coherent anti-Stokes Raman scattering

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Spontaneous Raman spectroscopy (SR) is a broadly used and versatile method for the analysis of structures in crystalline materials, such as strain distributions or ferroelectric domain walls. A large disadvantage of this technique are the high acquisition times of up to several seconds per data point to visualize these structures. In this work, we highlight the use of a promising alternative, broadband coherent anti-Stokes Raman scattering (B-CARS) and compare this technique with SR at the example of poled Lithium niobate. We demonstrate a more than 100 times higher signal-to noise ratio, while maintaining similar intensities. These results promise the use of BCARS for high-speed spectral imaging in the context of solid-state materials, such as ferroelectrics and their domain walls.

Investigating the magnetic properties of $BaCo_2(AsO_4)_2$: Magnetisation steps and Hamiltonian simulation

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We report on the observation of new magnetisation steps at very low temperature in the antiferromagnetic material $BaCo_2(AsO_4)_2$, which magnetic structure is still an enigma since the first works 40 years ago [1] and continues to be debated [2].

By combining neutron scattering measurements, spin wave and Monte Carlo simulations, we found a classical Heisenberg Hamiltonian with interactions up to the fourth nearest neighbours, which partially reproduces the spin waves dispersion observed in our experiment. We have synthesised substituted samples to test the effect of chemical pressure and the influence of the magnetic dilution on the propagation vector of $BaCo_2(AsO_4)_2$. These results are a step forwards identifying the magnetic structure of this compound.

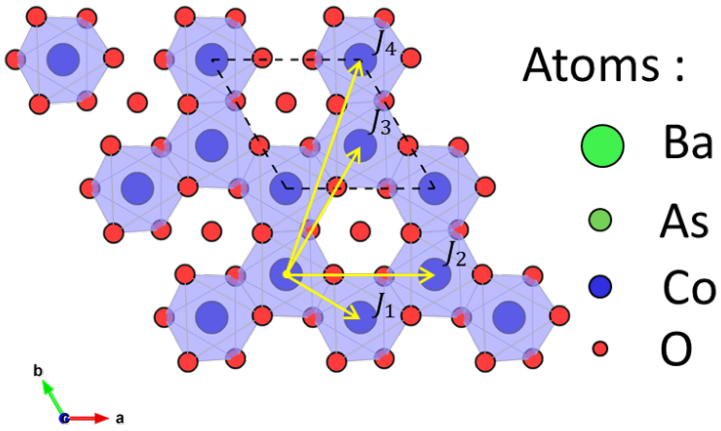

Figure 1: Honeycomb lattice of with the fourth magnetic interaction of the system $BaCo_2(AsO_4)_2$.

[1] L.-P. Regnault *et al.*, J. Phys. Soc. Jpn. **52** (Suppl.), 1 (1983).

[2] R. Zhong, T. Gao, N. P. Ong, and R. J. Cava, Sci. Adv. **6**, 1 (2020).

Photo-induced transport properties of ferroelectric domains and domain walls in lithium niobate single crystals

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Ferroelectric materials exhibit a spontaneous and stable dielectric polarization, resulting in a rich and variable assembly of domain and domain wall structures that is receiving continued attention [1,2]. Furthermore, the multifield-controlled (electrical, mechanical, optical) electrical transport across these crystals offers many prospects for the vivid application of ferroelectrics into electronic devices, such as ferroelectric sensors, memories, and even ferroelectric synaptic circuits [3-5]. Notably, (external) control of the electronic transport by means of photons is very desirable since being non-invasive and ultrafast, but has been studied only sparsely so far. In particular, polarization switching of domains and domain walls, band gap modulation, or domain wall dynamics, all are susceptible to the photon-electron interaction, and thus need fundamental and profound investigations as basis for further application.

In this work, we combine local-scale scanning probe techniques with analyzing the impact of light irradiation onto lithium niobate domains and domain walls, and vary both intensity and wavelength to probe their (local) electronic conductivity. On this basis, we can also realize the configuration of high density domain pattern arrays and modulate the domain wall conductivity through scanning probe microscopy and the assistance of UV light. Then, we demonstrate that the enhancement of transport properties and the switching behavior of lithium niobate domain walls can be regulated by illumination adjacent to the band gap. This multi-method approach thus will improve our in-depth knowledge on the local band structure and energy level distribution within domain walls, and will lay the foundation to design integrated nano-electro-optical components thereof.

[1] D. Meier, *et al.*, Nat. Rev. Mater. **7**, 157 (2022).

[2] D. M. Evans, *et al.*, Phys. Sci. Rev. **5**, 9 (2020).

[3] C. Godau, *et al.*, ACS Nano **11**, 5 (2017).

[4] E. Singh, *et al.*, Phys. Rev. B **106**, 144103 (2022).

[5] Z. D. Luo, *et al.*, ACS Nano **14**, 746 (2020).

The Role of Pre-Nucleation Clusters in C-S-H Nucleation

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Although cement is the most widely used construction material in the world, and the C-S-H gel is the most important phase in the cement paste, many questions about C-S-H nucleation at the atomic scale remain unanswered. Its formation is governed by a non-classical nucleation process which involves several steps. It is known that the intermediate step in nucleation corresponds to a dense phase, but the mechanism of the nucleation within the dense liquid-like phase it largely unknown at the atomic level [1, 2].

In this work, we evaluate the role that pre-nucleation clusters (PNCs) could play in C-S-H nucleation. Evolutionary algorithms together with density functional theory (DFT) are used to find the energetically best C-S-H clusters for different stoichiometries. The study covers a range from small clusters of one Ca and one Si atoms up to complexes of 4 Ca and 4 Si atoms. Among all the clusters, it is remarkable the presence of one complex very similar to a tobermorite building block. The energy of collected clusters are further minimized using DFT and a continuous solvation model, and the calculation of the formation free energies for the transitions between the clusters allows us to propose a formation mechanism of the PNCs.

Finally, the aggregation of the tobermorite-like clusters is studied be means of molecular dynamics and compared with experimental radial distribution functions of different stages of C-S-H hydration. It is found that the tobermorite-like clusters start to aggregate to form a structure similar to a tobermorite sheet. Moreover, it is found that these aggregated clusters already contain the short-order features of the C-S-H radial distribution function.

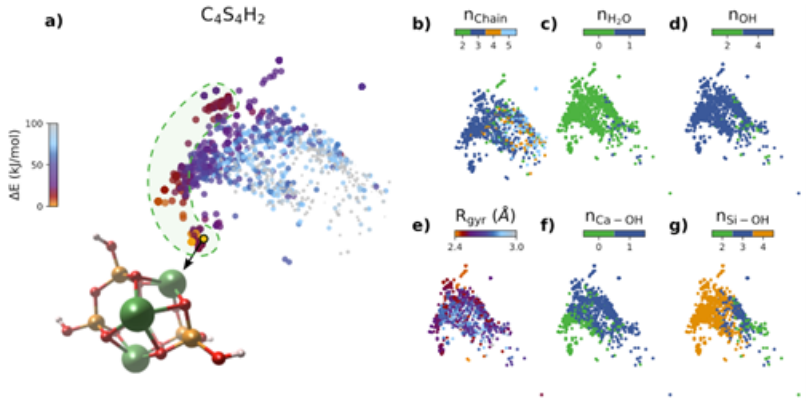

Figure 1: Sketchmap of the $C_4S_4H_2$ clusters where the colormap represent different properties in each image. Each dot represents a structure and the distance between points represents the structural distance between structures.

[1] Aretxabaleta, X. M., López-Zorrilla, J., Labbez, C., Etxebarria, I., and Manzano, H., *A potential CSH nucleation mechanism: atomistic simulations of the portlandite to CSH transformation*, Cement and Concrete Research **162**, 106965 (2022).

[2] Krautwurst, N., Nicoleau, L., Dietzsch, M., Lieberwirth, I., Labbez, C., Fernandez-Martinez, A., ... and Tremel, W., *Two-step nucleation process of calcium silicate hydrate, the nanobrick of cement*, Chemistry of Materials **30**(9), 2895–2904 (2018).

Machine Learning atomic potential for C-S-H

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Atomic-scale simulations are a powerful tool to understand and characterize materials and even design new ones with specific properties. However, simulating large systems with accurate methods is usually prohibitive, and most computational works on those materials rely on less accurate classical force fields. That is the case for cement-based materials, for which several classical force fields have been developed over the years [1].

Machine Learning potentials (MLPs) [2] provide a tool to enable such simulations with high accuracy but with several orders of magnitude lower computational impact, thus allowing the simulation of large complex systems with quantum physical accuracy. The potential is trained in a dataset of Density Functional Theory (DFT) calculations for the desired system and it can afterward be employed to predict the energy and forces of new structures not present on that set. Most importantly, this method allows training the potential in small systems and then using it to predict the properties of larger ones.

In this work, we present a dataset of DFT calculations for bulk systems containing combinations of the four main elements present in cement: Ca/Si/O/H. This set includes liquid and solid water, several polymorphs of silicon oxides and calcium oxides, 9-, 11- and 14-tobermorites, alite, belite and several small C-S-H models. Taking this set of calculations as a starting point, we construct and test a MLP for those systems with a particular focus on C-S-H gels. We showcase its ability to predict several elastic properties of those materials and its power to simulate larger C-S-H models. Ultimately, this work provides a highly accurate and efficient tool to simulate large-scale cement phases.

[1] Mishra, R. K., et al., *cemff: A force field database for cementitious materials including validations, applications and opportunities*, Cement and Concrete Research **102**, 68–89 (2017).

[2] Behler, J., *Neural network potential-energy surfaces in chemistry: a tool for large-scale simulations*, Physical Chemistry Chemical Physics **13**(40), 17930–17955 (2011).

Far-field and near-field spectroscopy techniques in the IR, MIR, and THz frequency regimes

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Ultrafast examination of the physical properties and dynamic phenomena in materials has been of great interest and ongoing development for many decades, with the goal to achieve a fundamental understanding of matter and more advanced technological systems. Here we introduce the state-of-the-art tools that are available in our laboratories at TU Dresden, for conducting macroscopic and nanoscopic examinations of materials over broadband frequency ranges (IR, MIR, and THz).

Our THz time-domain spectroscopy system (Fig. 1a) allows for the far-field spectroscopic evaluation of materials and the extraction of the physical properties in the THz frequency range (0.1–10 THz) [1]. In addition, the system allows for investigating the emission power and detection sensitivity of THz sources and detectors. On the nanoscale range, we apply cutting-edge technologies to investigate and examine materials in the spatial and temporal domains over the IR, MIR, and THz frequency regimes. Using scattering scanning near-field optical microscopy (s-SNOM) and nano-FTIR techniques (Fig. 1b), the physical and dynamic properties of materials can be extracted with a resolution as low as 10 nm (according to the radius of the tip apex) [2]. Nano pump-probe experiments can also be performed to measure the ultrafast physical dynamics in the time-domain. Our nanoscopic systems are combined with unique narrowband and broadband light sources providing excitation wavelengths from 650 nm to 15 µm as well as with accelerator-based THz sources (0.1–3 THz for TELBE and 1.2–60 THz for FELBE).

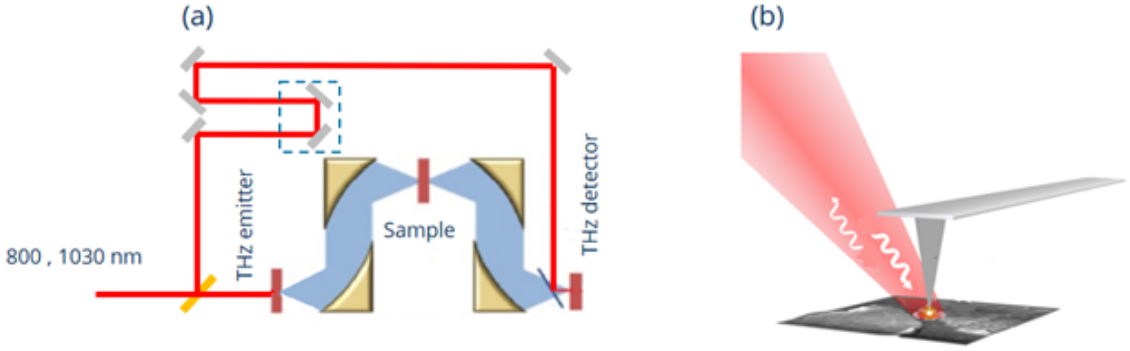

Figure 1: (a) THz time-domain spectroscopy system (THz-TDS), and (b) scattering scanning near-field microscopy (s-SNOM) for nanoscale spectroscopy and imaging.

[1] O. Hatem, *Peak emission of terahertz waves from (110)-oriented ZnTe by interacting phase-matched phonon resonances*, J. Opt. Soc. of Am. B **36**, 1144 (2019).

[2] T.V.A.G. Oliveira et al., *Nanoscale-Confined Terahertz Polaritons in a van der Waals Crystal*, Adv. Mater. **33**, 2005777 (2021).

Nanoscopic Investigation of the Monolayer $MoSe_2$ -WSe_2 Lateral Heterostructures under Illumination

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Transition metal dichalcogenides (TMDCs) such as $MoSe_2$ and WSe_2, are inorganic semiconductor monolayers with great potential for integration into nanoscale devices. Monolayers of different TMDCs can be engineered into lateral or vertical heterostructures forming, e.g., 1D or 2D p-n junctions that strongly respond to light [1]. Here, lateral heterostructures of monolayer $MoSe_2$ and WSe_2 grown by chemical vapor deposition are studied at the nanometer length scale by Kelvin Probe Force Microscopy (KPFM) under visible to near-infrared light illumination, i.e. photon energies between 1.45 and 1.95 eV. This approach enables for the simultaneous recording of both the sample surface morphology and the local photoinduced surface potential. By employing the side-band KPFM demodulation [2], quantification of the local band-bending of this in-plane heterostructure is possible with superior sensitivity. Different alterations of the local surface potential are observed when choosing the light exposure above and below the individual TMDCs bandgap energies.

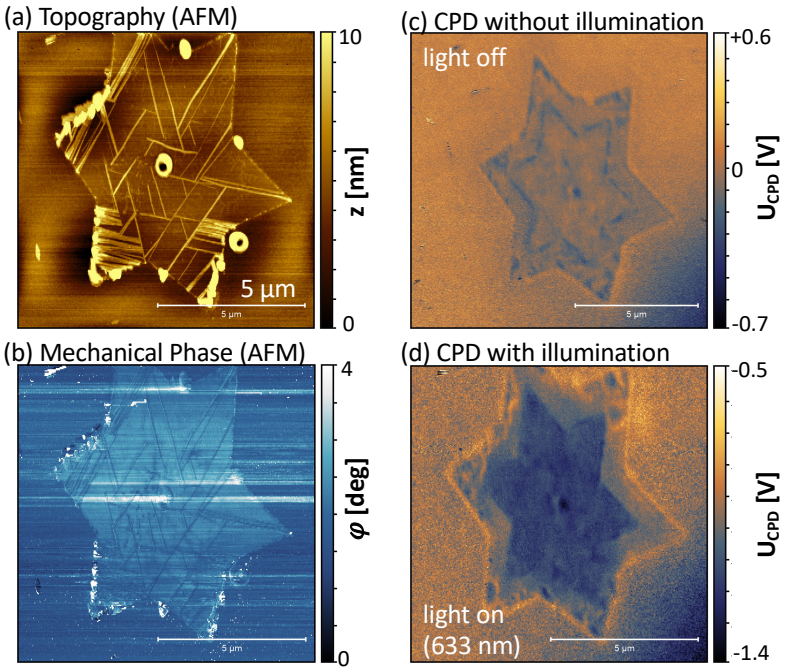

Figure 1: Nanoscopic study of 2D $MoSe_2$-WSe_2 lateral heterostructures with and without illlumination. (a,b) Topography and mechanical phase of the structures showing the star-like monolayer. (c-d) Imaging of the local contact potential difference (CPD) without (c) and with (d) illumination via a HeNe laser at 1.96 eV (above bandgap).

[1] P.A. Markeev *et al.*, J. Phys. Chem. C. **125**, 13551 (2021).
[2] T. Wagner *et al.*, Beilstein J. Nanotechnol. **6**, 2193 (2015).

The Impact of Schottky Barriers When Electrically Contacting Conductive Domain Walls in Lithium Niobate Single Crystals

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Conductive domain walls (DWs) in lithium niobate are promising constituents for applications in nanoelectronics, due to their high conductance [1] and ability to be created quasi-on-will through high-voltage poling. However, electrically contacting the DWs leads to the formation of a Schottky barrier between the DW and the electrode material [2].

In this work, we study a variety of different factors affecting the electronic transport across the barrier, e.g., the electrode material, the quality of the lithium niobate surface, and the influence of the applied voltages during the DW conductivity-enhancement procedure. It was found that all these factors significantly impact the Schottky barrier formation; moreover, the structure of the DW inside the bulk is also influenced by the electronic interface states. Our results underline the importance of providing reproducible sample surface conditions prior to sample poling, but identify promising directions for implementing an improved DW conductivity.

[1] Ch. Godau *et al.*, ACS Nano **11**, 4816 (2017).

[2] M. Zahn *et al.*, arXiv:2307.10322 [cond-mat.mtrl-sci]

Orientational ordering of water molecules confined in beryl: Molecular dynamics simulations

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Recent nuclear magnetic resonance (NMR) experiments on beryl crystals with confined water molecules have provided valuable insights into their behavior [1]. Building upon these findings, our research focuses on developing an improved model to analyze the interactions among water molecules' dipole moments [2]. The proposed model incorporates a local crystal potential featuring dihexagonal symmetry, which governs the rotations of water dipole moments, leading to their deflection from the *ab* hexagonal crystallographic plane.

The unique potential shape gives rise to intriguing consequences, particularly regarding the ordering of the dipole moments. Of special interest is the non-zero projection of the dipole moment along the hexagonal *c* axis. Our investigation aims to unveil the underlying tendency of water molecule dipoles toward an ordered phase within the beryl cage.

To accomplish this, we conduct molecular dynamics simulations to study the low-temperature behavior of confined water molecules in the beryl crystal lattice. Through our simulations, we explore the dynamical behavior of the water dipoles and gain insights into their tendency for ordering at lower temperatures.

[1] V. Chlan et. al., *Orientation and dynamics of water molecules in beryl*, J. Chem. Phys. **158**, 124308 (2023).
https://doi.org/10.1063/5.0131510

[2] A. Klic, V. Janis, and F. Kadlec, *Orientational ordering of water molecules confined in beryl: A theoretical study*, Preprint (2023).
arXiv:2303.15304 [cond-mat.mtrl-sci]

MP_tools: from molecular dynamics simulations to diffuse scattering maps

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To extract information on disordered structures from scattering data one often has to compare model-based scattering intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism.

With this progress in place the bottleneck has shifted from producing supercell models to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue was due to the fact that scattering amplitudes from a distorted lattice could not be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor $\exp(\mathrm{i}\boldsymbol{QR})$ being $\boldsymbol{Q}$-dependent.

As a consequence, many efforts in recent years have been restricted to simple models on small supercells [1, 2] or to more involved pair distribution function (PDF) analysis [3, 4, 5], where the summation problem is reduced to a single dimension. Nevertheless, the efficiency of PDF model generation in direct space for large supercells and large correlation distances needed for good quality Fourier transforms was limited by the radial distribution function spherical shells volume diverging with r^2.

The *MP_tools* program suite [6] addresses these issues employing innovative algorithms. In the first case, recent developments of the non-uniform fast Fourier transform [7] permit to accelerate the summation of scattering amplitudes from large supercells by orders of magnitude, bringing in the usual FFT speed and allowing for interactive work even in case of dynamic scattering functions $S(Q,\omega)$ based on time sequences of thousands of frames. A similar effect in the PDF accumulation brings a Monte-Carlo algorithm with projective sampling [8], permitting to accumulate the $g(r)$ pair-distribution function with uniform (r-independent) accuracy while bypassing the radial distribution function.

Many motivating discussions with M. Pasciak, P. Ondrejkovic and J. Hlinka from the Institute of Physics (AS CR, Prague) are kindly acknowledged.

[1] Welberry, T.R., Butler, B., J. Appl. Cryst. **27**, 205–231 (1994).

[2] Neder, R.B., Proffen, Th., *Diffuse Scattering and Defect Structure Simulations: A cook book using the program DISCUS*, Oxford (2008); https://doi.org/10.1093/acprof:oso/9780199233694.001.0001text

[3] McGreevy, R.L., J. Phys.: Condens. Matter **13**, R877–R913 (2001).

[4] Proffen, Th. *et al.*, Z. Kristallogr. **218**, 132–143 (2003).

[5] Eremenko, M. *et al.*, Nat. Commun. **10**, 2728 (2019).

[6] Kulda, J., https://github.com/jkulda/MP_tools, https://mptools.fr

[7] Barnett, A.H. *et al.*, J. Sci. Comput. **41**, C479–C504 (2019); https://github.com/flatironinstitute/finufft

[8] Kulda, J., Acta Cryst. A, in preparation (2023).

Terahertz Twistoptics – engineering canalized phonon polaritons

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The terahertz (THz) frequency range is key to study collective excitations in many crystals and organic molecules. However, due to the large wavelength of THz radiation, the local probing of these excitations in smaller crystalline structures or few-molecular arrangements, requires sophisticated methods to confine THz light down to the nanometer length scale, as well as to manipulate such a confined radiation. For this purpose, in recent years, taking advantage of hyperbolic phonon polaritons (HPhP) in highly anisotropic van der Waals (vdW) materials has emerged as a promising approach [1], offering a multitude of manipulation options such as control over the wavefront shape and propagation direction. Here, we demonstrate the first THz application of twist-angle-induced HPhP manipulation [2], designing the propagation of confined THz radiation between 8.39 and 8.98 THz in the vdW material alpha-molybdenum trioxide (α-MoO_3) [3], hence extending twistoptics to this intriguing frequency range. Our images, recorded by near-field optical microscopy, show the frequency- and twist-angle-dependent change between hyperbolic and elliptic polariton propagation, revealing a polaritonic transition at THz requencies. As a result, we are able to allocate canalization (highly collimated propagation) of confined THz radiation by carefully adjusting these two parameters, i.e., frequency and twist angle. Specifically, we report polariton canalization in α-MoO_3 at 8.67 THz for a twist angle of 50 °. Our results demonstrate an unprecedented control and the manipulation of highly-confined collective excitations at THz frequencies, offering novel possibilities for nanophotonic applications.

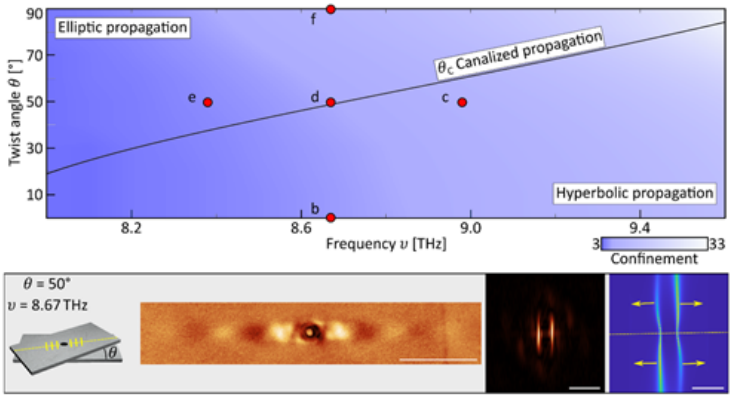

Figure 1: Upper part: Twist angle θ_C for canalized HPhPs propagation in the THz range as a function of frequency. The line separates elliptic and hyperbolic propagation regimes. The color scale depicts the predicted polariton confinement, assuming a stack of two 100 nm thick layers of α-MoO_3. Lower part: s-SNOM amplitude image taken at ν=8.67 THz for θ=50 °. Sketches of the TBLs and experimental/theoretical iso-frequency curves (IFCs) are shown to the left and right, respectively. Scale bars: 5 µm for real-space, 40 k_0 and 20 k_0 for the experimental and theoretical IFCs, respectively.

[1] D. N. Basov et al., *Polaritons in van der Waals materials*, Science **354**, 6309 (2016).

[2] G. Hu et al., *Topological Polaritons and Photonic Magic Angles in Twisted α-MoO_3 Bilayers*, Nature **582**, 209 (2020).

[3] T.V.A.G. de Oliveira et al., *Nanoscale-Confined Terahertz Polaritons in a van der Waals Crystal*, Adv. Mater. **33**, 2005777 (2021).

Time-resolved s-SNOM on single GaAs-InGaAs nanowires

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Contactless investigation of the charge carrier concentration and mobility on individual nanowires (NWs) by scattering-type scanning near-field optical microscopy (s-SNOM) provides a spatial resolution far beyond the diffraction limit. Utilizing near-infrared (NIR) excitation on (typically intrinsic) NWs, charge carrier lifetimes become accessible in NIR-pump / THz-probe experiments in the far-field [1,2]. This pump-probe technique was recently combined with near-field microscopy, enabling investigations of the carrier dynamics on single InAs NWs [3].

Time-resolved near-field spectroscopy studies are still missing for doped nanowires, where existing free electrons can gain additional kinetic energy from THz radiation via intraband absorption. Here we report on THz-pump / MIR-probe s-SNOM studies on highly-doped GaAs/ InGaAs core-shell NWs utilizing the intense narrowband THz pulses from the free-electron laser FELBE.

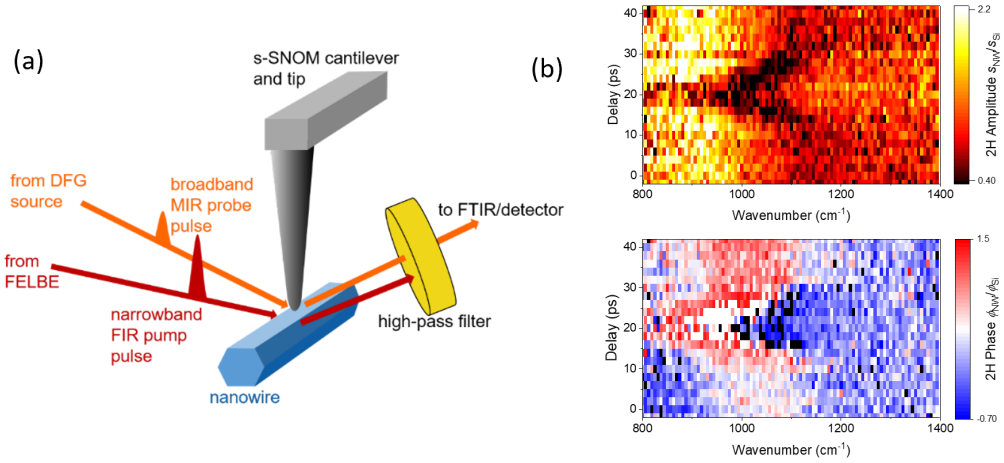

Figure 1: (a) Sketch of the THz-pump / MIR-probe nanospectroscopy experiment; (b) Near-field amplitude $s(\omega)$ and phase $\varphi(\omega)$ spectra (second harmonic of the tip modulation) as functions of the delay time between the THz-pump and the broadband MIR probe. The spectra are normalized to the response of a Si reference.

Results of the THz-pump / MIR-probe experiment are shown in Fig. 1(b). Upon intraband THz-pumping (12 THz / 400 cm^{-1}) we observe a red shift of the NW plasma resonance both in the amplitude and phase, which decays mono-exponentially with a time constant of t_{exp}=4.3±0.8 ps. We assign the observed red shift to a substantial heating of electrons in the conduction band and the subsequent increase of the effective mass at the nonparabolic Γ-valley and due to transfer to side valleys.

[1] H. J. Joyce et al., *Electronic properties of GaAs, InAs and InP nanowires studied by terahertz spectroscopy*, Nanotechnology **24**, 214006 (2013).
[2] I. Fotev et al., *Electron dynamics in $In_xGa_{1-x}As$ shells around GaAs nanowires probed by terahertz spectroscopy*, Nanotechnology **30**, 244004 (2019).
[3] M. Eisele et al., *Ultrafast multi-terahertz nano-spectroscopy with sub-cycle temporal resolution*, Nature Photonics **8**, 841-–845 (2014).

Towards 3-dimensional magnetic force microscopy (3D-MFM)

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Magnetic Force Microscopy (MFM) is a technique for recording maps of the magnetic stray field above a sample, as is for instance well documented for magnetic Bloch- [1, 2, 3] and Néel-type [4, 5] skyrmions, or so-called anti-skyrmions [6, 7]. In MFM, the magnetized tip usually couples to the out-of-plane magnetic sample stray field through cantilever oscillations perpendicular to the sample surface. Nevertheless, the stray field naturally has a fully 3-dimensional (3D) distribution, the reconstruction of which has not been widely performed so far due to the uniaxial sensitivity of standard MFM.

Here, we introduce a novel way towards experimentally mapping the full 3D sample stray field, by simultaneously oscillating the MFM cantilever at its vertical (out-of-plane) and lateral (in-plane) fundamental resonance frequencies, thus making it possible to directly compare and quantify the *vertical* MFM (V-MFM) and the *lateral* MFM (L-MFM) signals. We have tested this novel setup for its overall performance and signal-to-noise ratio, using two distinct samples: a hard disk with known magnetization and a Heusler MnPtPdSn sample [8] that exhibits complex 3D magnetic domain patterns. A good agreement was found between experimental results and numerical calculations for the known hard-disk magnetization.

[1] P. Milde *et al.*, Science **340**, 1076 (2013); https://doi.org/10.1126/science.1234657

[2] S. Zhang *et al.*, Nano Lett. **16**, 3285 (2016); https://doi.org/10.1021/acs.nanolett.6b00845

[3] P. Milde *et al.*, Phys. Rev. B **100**, 024408 (2019); https://doi.org/10.1103/PhysRevB.100.024408

[4] I. Kézsmárki *et al.*, Nat. Mater. **14**, 1116 (2015); https://doi.org/10.1038/nmat4402.

[5] E. Neuber *et al.*, J. Phys.: Cond. Matter **30**, 445402 (2018); https://doi.org/10.1088/1361-648X/aae448

[6] B.E. Zuniga Cespedes *et al.*, Phys. Rev. B **103**, 184411 (2021); https://doi.org/10.1103/PhysRevB.103.184411

[7] M. Winter *et al.*, Commun. Mater. **3**, 102 (2022); https://doi.org/10.1038/s43246-022-00323-6

[8] M. Hoffmann *et al.*, Nat. Commun. **8**, 308 (2017); https://doi.org/10.1038/s41467-017-00313-0.

Exfoliation of 2D Materials for NanoOptics

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The desire for smaller and more energy efficient optical components leads to the necessity of light confinement below the diffraction limit. This is achieved e.g by phonon polaritons (PhPs) which are quasi-particles formed by coupling infrared photons to optical phonons in a crystal. Particularly, the related light confinement is enhanced when the PhPs are generated in anisotropic, 2D van der Waals materials, such as MoO_3 and GeS [1, 2]. Hence, atomically-flat and µm-sized nano-sheets of such materials are required, as being readily realized through mechanical exfoliation [3].

Here, we present an optimized exfoliation technique allowing us to reproducibly prepare nano-sheets made up from MoO_3 and GeS with a lateral size of 20–100 µm and a 100–200-nm thickness (see Fig. 1). We present a quick and easy to implement adaptation of the *Scotch-tape* exfoliation technique as well as exemplary results based on scanning force microscopy and optical nanoscopy imaging.

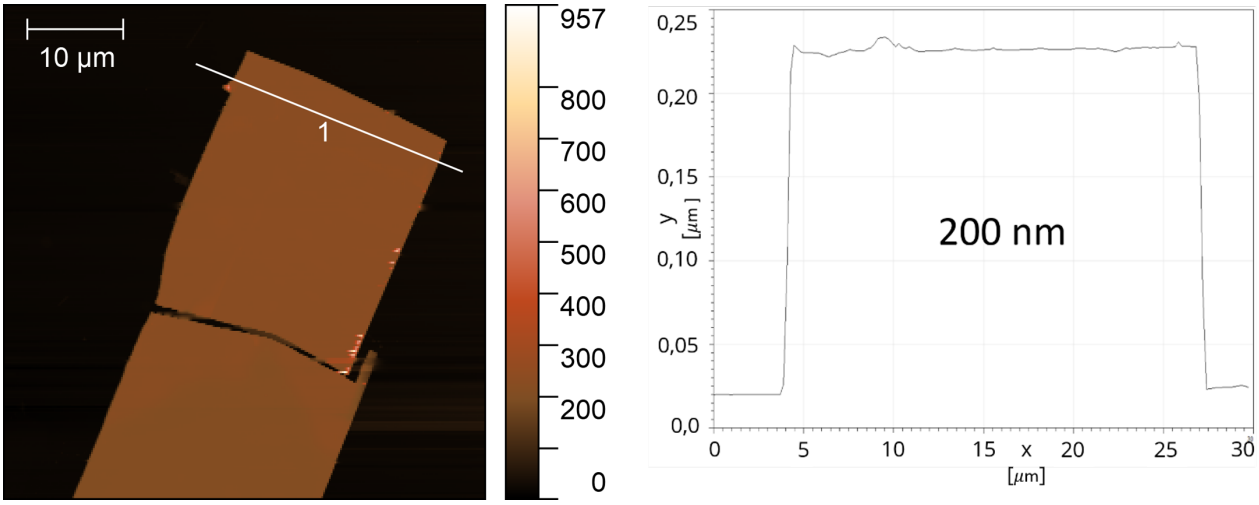

Figure 1: (a) Scanning force microscopy image of MoO_3 flake on Si and (b) the corresponding cross section along the line in (a).

[1] T.V.A.G. de Oliveira *et al.*, Adv. Mater. **33**, 2005777 (2021).

[2] T. Nörenberg *et al.*, ACS Nano **16**, 20174 (2022).

[3] X. Zhang *et al.*, 2D Mater. **8**, 032002 (2021).

Fabrication of Artificial Interfaces between the Ferroelectric Crystals

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Hetero-structures play an important role in the advancement of current physics and technology as they resulted not only in the discovery of novel physical phenomena but also offered quite an improvement in the properties of the devices, and a dream to create new materials – "manmade materials" – a reality [1, 2]. Ferroelectric materials like Lithium Niobate (LN) possess switchable electric polarization and non-linear optical characteristics. These traits make them highly useful in various fields, rendering them excellent contenders for creating heterostructures [3]. Though epitaxial growth techniques hold the potential for fabricating such structures by finely tuning growth parameters, their feasibility relies on several factors. These factors pose limitations to our choice of materials and prompt the need to look into other flexible technologies [4, 5]. In this work direct wafer bonding was tested to see if it is a potential solution to fabricate ferroelectric heterostructures. This work successfully demonstrates the fabrication of several LN homo-structures (Figure 1) with a simple bonding recipe. Several experiments were conducted to optimize the bonding recipe for obtaining better bond strength between the crystals. Furthermore, the electrical characterization of the fabricated LN homo-structures showed that their electrical properties were almost similar to the properties of homogeneous crystals proving the viability of direct wafer bonding technology for creating conductive devices.

The next phase would be to combine diverse ferroelectric materials and semiconductors and create hybrid ferroelectric heterostructures with "the best of both worlds" for novel applications and enhanced performance.

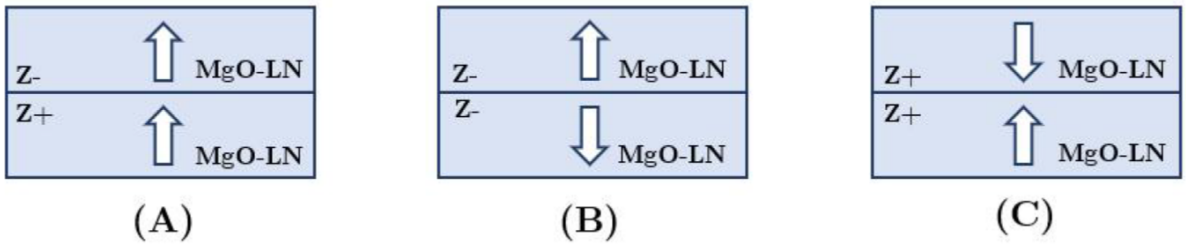

Figure 1: A two-dimensional (2-D) graphic picture of single-crystal Z-cut 5% Magnesium Oxide-doped Lithium Niobate (5% MgO-LN) homo-structures with (A) Z+/Z- interface, (B) Z-/Z- interface, and (C) Z+/Z+ interface. The arrows in the picture represent the orientation of the domains in the crystal structure.

[1] Alferov, Z. I., *Semiconductors* **32**, 1–14 (1998).

[2] Li, M. Y., Chen, C. H., Shi, Y., and Li, L. J., *Materials Today* **19**(6), 322–335 (2016).

[3] Bazzan, M., and Fontana, M., *Applied Physics Reviews* **2**(4), 1931–9401 (2015).

[4] Ahn, C. H., Rabe, K. M., and Triscone, J. M., *Science* **303**, 488–491 (2004).

[5] Schwarzkopf, J., and Fornari, R., *Progress in crystal growth and characterization of materials* **52**(3), 159–212 (2006).

Lattice dynamics and pressure-temperature phase diagram of candidate quantum paraelastic $BaZrO_3$

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$BaZrO_3$ is one of the rare perovskites that is claimed to remain cubic down to the lowest temperatures. In spite of this apparent simplicity, its exact structural details have been under debate due to a number of theoretical and experimental observations, most notably:

- the presence of a clear structural instability revealed by first-principle calculations, but extremely sensitive to a particular choice of functionals;
- the presence of a strong Raman spectrum where no first-order Raman scattering by phonons is in principle allowed;
- the possible presence in ceramic samples of dynamic nanodomains of a lower symmetry than the average cubic structure.

This situation has led to a number of hypothesis and open questions on the possible presence of those nano-domains, the variety of structural phase transitions occurring under hydrostatic pressure and the possible role of quantum fluctuations in the stabilization of the average cubic structure, which would make $BaZrO_3$ a "quantum paraelastic".

In this talk, I will summarize recent findings [1,2,3] on this system, largely made possible by the availability of single crystals.

[1] P. Rosander et al., *Anharmonicity of the antiferrodistortive soft mode in barium zirconate $BaZrO_3$*, Phys. Rev. B **108**, 014309 (2023).

[2] C. Toulouse et al., *Stability of the tetragonal phase of $BaZrO_3$ under high pressure*, Phys. Rev. B **106**, 064105 (2022).

[3] C. Toulouse et al., *Lattice dynamics and Raman spectrum of $BaZrO_3$ single crystals*, Phys. Rev. B **100**, 134102 (2019).

Antiferroelectric till next time: Raman and dielectric spectroscopy of $PbZrO_3$

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Antiferroelectrics have lately undergone an accrued interest, due to their high applicability as electrocaloric cooling [1] or energy storage devices [2]. However, much is still to be investigated on the fundamental structure and switching of these materials.

For instance, recent work has casted some doubts about the true ground state of canonical antiferroelectric perovskite lead zirconate ($PbZrO_2$), by proposing either an 80-atom *Pnam* cell [3] or a polar 30-atom *Iba2* structure [4] as ground state, instead of the currently commonly-accepted structure of $PbZrO_3$, which is an orthorhombic 40-atom cell with *Pbam* space group [5].

In this work, we present low-temperature Raman and dielectric spectroscopy to confirm or dispute the antiferroelectric nature of $PbZrO_3$ single crystals.

Single crystals with two different orientations (c-axis out-of-plane and c-axis in-plane) have been measured in every possible polariser and analyser orientation to access all symmetries of the Raman spectra. We observe no apparent phase transition from room temperature to 4 K and find that the measured spectra can be fully interpreted by the standard 40-atom *Pbam* space group. Raman results are compared to the different possible ground states by group theory analysis but also analysed with respect to phonon mode frequencies calculated by Density Functional Theory. These findings are confirmed by dielectric measurements that show no anomalies below room temperature.

[1] A. S. Mischenko, Q. Zhang, J. F. Scott, R. W. Whatmore, and N. D. Mathur, *Giant electrocaloric effect in thin-film* $PbZr_{0.95}Ti_{0.05}O_3$, Science **311**, 1270–1271 (2006).

[2] Z. Liu et al., *Antiferroelectrics for Energy Storage Applications: a Review*, Advanced Materials Technologies **3**, 1800111 (2018).

[3] J. S. Baker et al., *A re-examination of antiferroelectric* $PbZrO_3$ *and* $PbHfO_3$*: an 80-atom* Pnam *structure*, preprint available on: https://arxiv.org/abs/2102.08856v2 (2021).

[4] H. Aramberri, C. Cazorla, M. Stengel, and J. Íñiguez, *On the possibility that* $PbZrO_3$ *not be antiferroelectric*, npj Computational Materials **7**, 1–10 (2021).

[5] R. Kagimura and D. J. Singh, *First-principles investigations of elastic properties and energetics of antiferroelectric and ferroelectric phases of* $PbZrO_3$, Physical Review B **77**, 104113 (2008).

$BiFeO_3$ domain walls and nanodomains at low temperature

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We present a study of ferroelectric 180 ° domain walls in multiferroic $BiFeO_3$, a material in which two order parameters coexist. Therein the ferroelectric phase transition entails the emergence of polarization and antiphase rotations of the O octahedra. The interplay of the two distortions and the energies of various possible geometries of domain walls were studied before with the first-principle calculations by Diéguez et al. [1]. Here, using ab-initio based atomistic model for $BiFeO_3$ [2], we concentrate on the configuration of [111]pc and [-1-1-1]pc domains with two 180 ° domain walls separating them.

In contrast with the previous study [1], atomistic simulations allow to inspect also more complex nanodomain geometries, including those of antiskyrmions recently discovered in $BaTiO_3$ [3].

[1] O. Diéguez et al., *Domain walls in a perovskite oxide with two primary structural order parameters: first-principles study of $BiFeO_3$*, Phys. Rev. B **87**(2), 024102 (2013).

[2] M. Graf et al., *Development of an Atomic Level Model for $BiFeO_3$ from First-Principles*, Ferroelectrics **461**, 61 (2014).

[3] Mauro A. P. Gonçalves, Marek Paściak, and Jiří Hlinka, *Antiskyrmionic ferroelectric medium*, Preprint (2023). arXiv:2303.07389 [cond-mat.mtrl-sci]

Spatially resolved low-frequency dynamics of Ba(Zr,Ti)O_3

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Large-scale molecular dynamics simulations based on an effective Hamiltonian approach are used to calculate and predict macroscopic properties of various materials and their solid solutions. Recently, F. Mayer *et al.* [1] have elaborated on the theoretical description of substitution in effective Hamiltonians as well as their parametrization by density functional theory calculations for two model systems of relaxor ferroelectric materials: homovalent substituted $BaZr_xTi_{1-x}O_3$ (BZT100x) and heterovalent substituted $BaNb_xTi_{1-x}O_3$ (BNT100x). The effective Hamiltonian for BZT was used for benchmarking against other models and experimental data on the phase diagrams and dielectric properties. Subsequently, the effective Hamiltonian model was further extended and successfully used to parametrize BNT. To testify the predictive power of the developed BZT model, we have extensively utilized results of molecular dynamics simulations to explore lattice and relaxor dynamics of BZT.

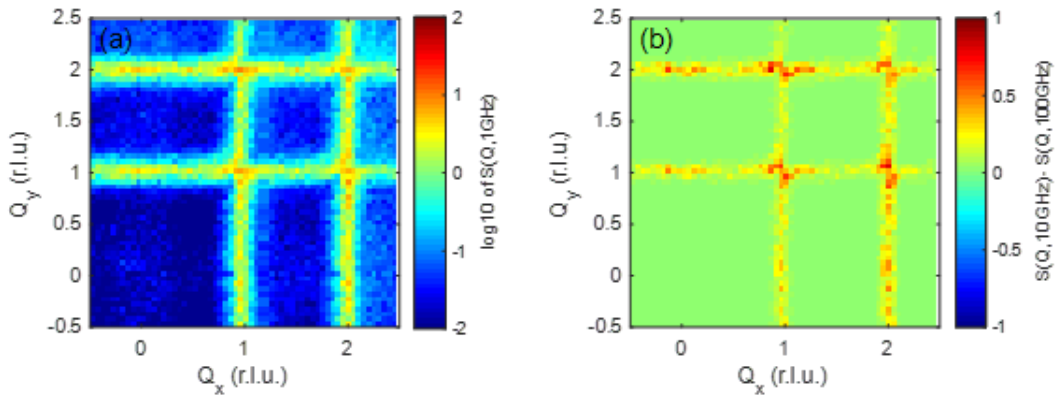

Figure 1: X-ray scattering in the (hk3/2) plane of the relaxor ferroelectric BZT40 at 150 K: (a) quasielastic scattering at 1 GHz and (b) an inelastic component obtained by subtracting inelastic scattering at 10 and 100 GHz. The energy resolution is 8 GHz.

We will present calculation of crystal structure from the effective Hamiltonian model of BZT and its (in)elastic x-ray scattering using the recently developed program *MP_tools* [2]. We will focus on lattice dynamics of ferroelectric $BaTiO_3$ and relaxor ferroelectric BZT40 and compare obtained results with atomistic models and experimental data [3]. Particularly, we will present spatially resolved low-frequency dynamics of the relaxor ferroelectric BZT40 (see Figure 1) in a wide frequency range from 1 GHz to 50 THz and address a novel insight into relaxor behavior of BZT.

[1] F. Mayer, M.N. Popov, P. Ondrejkovic, J. Hlinka, J. Spitaler, and M. Deluca, *Finite-temperature investigation of homovalent and heterovalent substituted $BaTiO_3$ from first principles*, Phys. Rev. B **106**, 224109 (2022).

[2] J. Kulda, Acta Cryst. A (2023) in preparation; https://mptools.fr

[3] M. Paściak, T.R. Welberry, J. Kulda, S. Leoni, and J. Hlinka, *Dynamic displacement disorder of cubic $BaTiO_3$*, Phys. Rev. Lett. **120**, 167601 (2018).

Orientational disorder and formation of ferroelastic textures in selected organometallic crystals

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Transparency of many organometallic crystals allows one to use the optical polarization microscopy to watch the formation and evolution of domains arising in phase transitions. The existence of domains follows from the Curie principle in instances of spontaneous symmetry breaking [1]. The latter reflects an interplay between a dynamic disorder of quasi-rigid molecular ions and the tendency of the whole system to reach a minimum of a thermodynamic potential in varying temperature. Structural data and symmetry considerations help to reveal mechanisms of molecular ordering, to predict the spatial orientation of ferroelastic domain walls [2, 3] and even their coloured vs colourless nature [4]. General scheme of symmetry breaking will be demonstrated. Examples of domain patterns and kinetics of their formation will be presented along with hypotheses concerning the details of the observed textures.

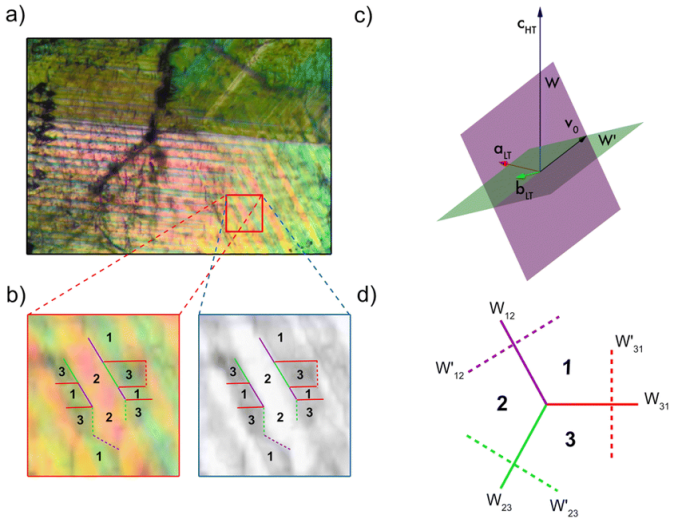

Figure 1: Coloured domain pattern of (azetidinium)$_2$(H_3O)[$Co(CN)_6$] withdomain walls oblique with respect to observation direction (here c_{HT}) [4].

[1] P. Curie, *Sur la symétrie dans les phénomènes physiques, symétrie d'un champ électrique et d'un champ magnétique*, Journal de Physique Théorique et Appliquée (in French). EDP Sciences **1**(3), 393–415 (1894). doi:10.1051/jphystap:018940030039300

[2] P. Szklarz, A. Pietraszko, R. Jakubas, G. Bator, P. Zieliński, and M. Gałazka, *Structure, phase transitions and molecular dynamics of [C(NH$_2$)$_3$]$_3$[M$_2$I$_9$], M = Sb, Bi*, J. Phys.: Condens. Matter **20**, 255221 (2008). doi:10.1088/0953-8984/20/25/255221

[3] M. Moskwa, E. Ganczar, P. Sobieszczyk, W. Medycki, P. Zieliński, R. Jakubas, and G. Bator, *Temperature-Stimulus Responsive Ferroelastic Molecular–Ionic Crystal: ($C_8H_{20}N$)[BF_4]*, J. Phys. Chem. C **124**, 18209–18 (2020). doi:10.1021/acs.jpcc.0c05322

[4] M. Moskwa, P. Sobieszczyk, J.W. Mikurenda, P. Zieliński, and M. Rok, *Improper ferroelastic phase transition in a hydrogen-bonded metallocyanide-based (azetidinium)$_2$(H_3O)[$Co(CN)_6$] framework*, Chem. Commun. **59**, 5535–5538 (2023). doi:10.1039/D3CC01253K

Wednesday, 27^{th} Sep 2023

Terahertz High Harmonics in Dirac Materials

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Dirac Materials, such as graphene and topological insulators, exhibit extremely strong interaction with terahertz (THz) radiation owing to the unique Dirac cone in the electronic band structure. Here, the linear dispersion relation allows for instantaneous carrier acceleration by strong THz field transients, enabling ultrafast heating of the electronic system to several 1000s of Kelvin. The resulting highly nonlinear light-matter interaction leads to the generation of high harmonics in the THz range (THz-HHG) with unprecedented conversion efficiencies [1]. This frequency upconversion process can be tuned by a variety of means, e.g. electrochemical gating or metallic antenna structures [2], and it is shown that even graphite from pencil drawings exhibits strong THz nonlinearities [3]. We demonstrate that using a phenomenological thermodynamic model, the properties of different Dirac (meta)materials can be described comprehensively. Making use of the imbalance of fs to ps timescales between THz-heating, thermalization and subsequent carrier cooling we find design principles for creating THz frequency converters with record efficiencies up to 8% in THz field. We further demonstrate that THz-HHG even extends to ultrafast emission in the optical and UV ranges of the electromagnetic spectrum potentially enabling THz-to-optical conversion for high speed data links [4].

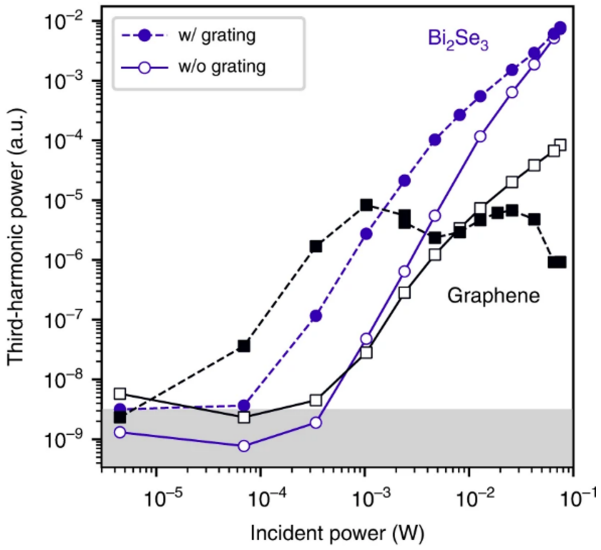

Figure 1: Plot of measured THz third harmonic conversion efficiencies for different material systems as a function of fundamental power showing the record conversion efficiency in topological insulators.

[1] H. A. Hafez, S. Kovalev, J.-C. Deinert et al., *Extremely efficient terahertz high-harmonic generation in graphene by hot Dirac fermions*, Nature **561**, 507–511 (2018).

[2] J.-C. Deinert et al., *Grating-graphene metamaterial as a platform for terahertz nonlinear photonics*, ACS Nano **15**, 1145–1154 (2021).

[3] A. Arshad et al., *Terahertz Harmonic Generation from Graphite Pencil Drawings*, Adv. Photon. Res. **4**, 2300088 (2023).

[4] I. Ilyakov et al., *Ultrafast Tunable Terahertz-to-Visible Light Conversion through Thermal Radiation from Graphene Metamaterials*, Nano Lett. **23**, 3872–3878 (2023).

Higgs-Spectroscopy in Superconductors

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High field THz-pulses allow accessing the Higgs mode, the amplitude mode of the order parameter, in superconductors. Using a phase-resolved THz-high-harmonics-spectroscopy allows performing a complex Higgs-spectroscopy of the order parameter dynamics, symmetry and interaction with other collective modes [1, 2]. In high-T_c cuprates and $NbSe_2$ this allows investigating the interplay of charge density waves (fluctuations) and superconductivity based on a generalised Fano-interference of the driven order parameters [1, 3, 4]. As time-resolved technique THz-Higgs spectroscopy also allows probing transient superconducting states driven by ultrashort light pulses [5, 6]. In these the phase sensitive measurement technique allows applying a 2D THz-third harmonics spectroscopy to disentangle different sources of third harmonics generation and describe their interplay [6]. As such Higgs spectroscopy could become both a probe of superconducting condensates in and out of equilibrium and transient Higgs modes could serve as novel criterion for light driven transient superconducting states.

[1] H. Chu et al., *Nat. Commun.* **11**, 1793 (2020).

[2] L. Schwarz et al., *Nat. Commun.* **11**, 287 (2020).

[3] H. Cu et al., *Nat. Commun.* **14**, 1343 (2023).

[4] L. Feng et al., arXiv:2211.10947v2 [cond-mat.supr-con]

[5] K. Katsumi et al., *Phys. Rev. B* **107**, 214506 (2023).

[6] M. Kim et al., arXiv:2303.03288v1 [cond-mat.supr-con]

Dynamic structural instabilities in Halide perovskites and their relation to their opto-electronic properties

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Halide perovskites exhibit outstanding opto-electronic properties e.g. long carrier lifetime and low defect densities. They have been attracting attention due to their solar power conversion efficiencies (surpassing sometimes 30%) outperform those of traditional materials such as silicon and therefore may well determine the future of photovoltaics.

It is well known that the dynamic structural instabilities in these materials are ubiquitous – in the Raman spectrum they even show anharmonic thermal fluctuations resulting in diffuse inelastic scattering that increases towards 0 cm^{-1}, which is usually the signature of a liquid [1]. This suggests that they could be associated with opto-electronic properties, but unfortunately previous attempts link dynamic structural instabilities to the opto-electronic properties have been incomplete [2, 3]. In our fundamental theoretical work, we introduce the concept of dynamic tilting based on a number of well-documented characteristic experimental signatures [4]. We show how dynamically unstable materials can be stabilized at $T > 0$, how this can give rise to new crystal symmetries in perovskites, and most importantly, how these dynamical instabilities can explain important properties of highly efficient photovoltaic materials.

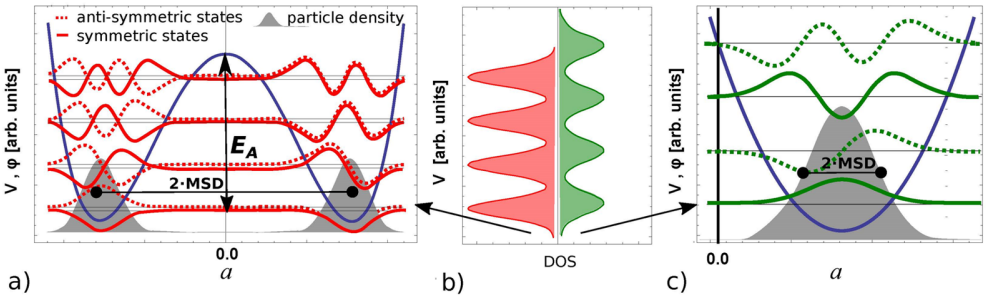

Figure 1: A schematic illustration of the possible shape of potential energy surface $V(a)$ as a function of the octahedral rotational angle in a perovskite. (a) Dynamic tilting due to a double-well potential $V(a)$ (blue). Resulting ionic wave functions $\Psi(a)$ are indicated in red and show two distinct localizations in both potential minima and so does the particle density $|\Psi(a)|^2$ (shaded in grey). The average tilting angle still remains at $a = 0$. The particle density is split and thus can explain large atomic displacements. (b) Comparison of the vibrational DOS (smearing applied for better visibility). The energy spectrum is particularly dense for the double well, due to almost degeneracy of these energy states. This gives rise to small transition energies and thus potentially to *large polarizability*. (c) Static tilting due to a single potential with a minimum at $a \neq 0$. The resulting ionic wave function $\Psi(a)$ with the lowest energy shows a single localization at the minimum of $V(a)$. From Ref. [4].

[1] Gao, L., et al., *Metal cation's lone-pairs increase octahedral tilting instabilities in halide perovskites*, Mater. Adv. **2**, 4610–4616 (2021).

[2] Steele, J.A., et al., *Role of electron–phonon coupling in the thermal evolution of bulk rashba-like spin-split lead halide perovskites exhibiting dual-band photoluminescence*, ACS Energy Lett. **4**, 2205–2212 (2019).

[3] Marronnier, A., et al. *Structural instabilities related to highly anharmonic phonons in halide perovskites*, J. Phys. Chem. Lett. **8**, 2659–2665 (2017).

[4] Adams, D. J., and Churakov, S. V., *Classification of perovskite structural types with dynamical octahedral tilting*, IUCrJ **10**, 309–320 (2023).

Phonon Polaritons in Low-Symmetry Crystals

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Surface phonon polaritons, light-matter coupled waves at the interface between a dielectric and a polar crystal, have recently attracted much attention as a versatile tool for low-loss nanophotonic applications in a range spanning from mid- to far-infrared [1]. These modes emerge inside the Reststrahlen band, i.e., the spectral region between the transverse and longitudinal optical phonon frequencies where the dielectric permittivity is negative. Particularly exotic polaritonic modes have recently been observed for strongly anisotropic crystals, where hyperbolic polaritons emerge naturally, featuring extreme light confinement, strongly directional propagating and high density of photonic states [2].

For lowest-symmetry monoclinic and triclinic crystals, we recently discovered hyperbolic shear polaritons [3] which exhibit an additional symmetry breaking of the nanoscale polariton propagation due to optical shear forces. We could also show that we can control the degree of shear polariton symmetry breaking by optically coupling to different polariton momentum components [4], see Figure 1. Furthermore, we were able to uncover a new form of polaritons at strongly anisotropy crystals interfaces, where radiation leakage into ordinary bulk states leads to hybrid interface-bound states, so-called leaky polariton modes [5].

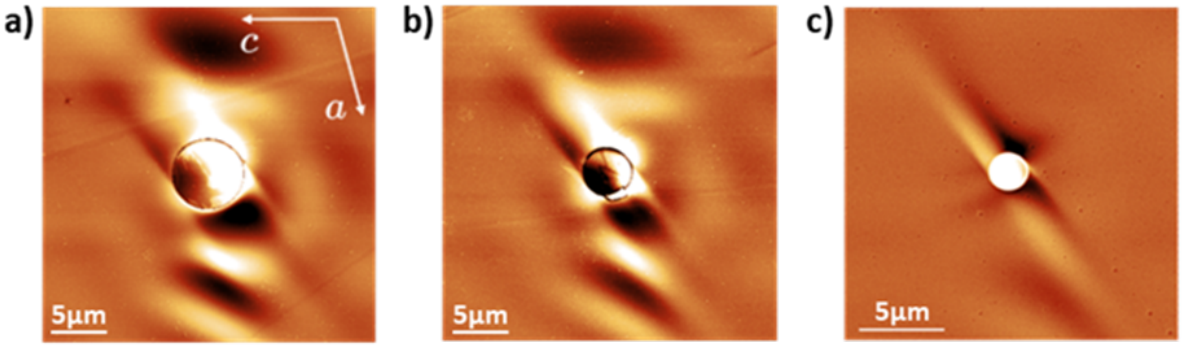

Figure 1: Optical near-field images of hyperbolic shear polaritons at the β-Ga_2O_3 surface, launched by decreasing-size (a-c) circular gold nano-antennas, leading to an increasing polariton propagation asymmetry [4].

[1] J. D. Caldwell, et al., *Low-loss, infrared and terahertz nanophotonics using surface phonon polaritons*, Nanophotonics **4**, 44 (2015).

[2] D. N. Basov, et al., *Polariton Panorama*, Nanophotonics **10**, 549 (2021).

[3] N. C. Passler, et al., *Hyperbolic Shear Polaritons in Low-Symmetry Crystals*, Nature **602**, 595 (2022).

[4] J. Matson, et. al, *Controlling the Propagation Asymmetry of Hyperbolic Shear Polaritons in Beta-Gallium Oxide*, Nature Communications, accepted (2023).
https://doi.org/10.21203/rs.3.rs-2365178/v1

[5] X. Ni, et al., *Observation of directional leaky polaritons at anisotropic crystal interfaces*, Nature Communications **14**, 2845 (2023).

Molecular motions in electrospun polymer/pharmaceutical drug fibers

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In recent years, there has been significant interest in the use of electrospun fibers as systems for delivering drugs, primarily due to their large surface area, ability to adjust their shape, and the diameter of the fibers. One key advantage of drug-loaded fibers is their capacity to regulate the release of drugs based on the composition and structure of the fibers.

These studies primarily focus on investigating the molecular dynamics (molecular relaxation processes) of polycaprolactone (PCL) fibers that contain different weight percentages of ornidazole (ORN), as well as core–shell structured fibers composed of amphiphilic poly(2-vinyl pyridine-co-styrene) (P2VP-PS) as the shell and a blend of PCL with ORN as the core. ORN exhibits a significantly higher glass transition temperature (T_g=277 K) compared to PCL (T_g=209 K). The PCL/ORN fibers behave as miscible blends, and Differential Scanning Calorimetry (DSC) measurements reveal a single glass transition that depends on the concentration of the drug in the system. Broadband dielectric spectroscopy (BDS) analysis of the PCL/ORN fibers identifies three relaxation processes: i) the α-relaxation process resulting from the fluctuation of PCL segments, ii) the secondary β-relaxation of PCL, and iii) a slow relaxation process at high temperatures attributed to hydrogen bonding between PCL and ORN. The β-relaxation of the PCL component remains unaffected by the presence of ORN molecules, while the other two processes are sensitive to the composition. In this contribution, we will discuss the impact of ORN content and the fiber shell on the glass transition temperature and molecular dynamics of PCL/ORN fibers and PCL/ORN core. Finally, we will present the kinetics of drug release from fibers monitored by UV-vis measurements.

Vibrational signatures of ferroelectric domain walls and knots

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This contribution aims to overview the emerging field of exploration of the lattice excitations associated with the topological defects in ferroelectric crystal lattices. Particular attention will be payed to the internal vibrations of supercrystals formed by ferroelectric domain walls [1,2], ferroelectric vortices [3], ferroelectric skyrmions [4] and antiskyrmions [5]. The presentation will focus on the the general outline of the field and conceptual problems and technical theoretical and experimental challenges. A recent specific example addressing the experiment-driven atomistic modeling study of ferroelectric bubble skyrmions in $PbTiO_3/SrTiO_3$ superlattice will be described in details at this symposium by a colleague of mine [4].

I would like to acknowledge inspirations from calculations and insights of my colleagues from the Department of Dielectrics, in particular that of M. Paściak, P. Ondrejkovič, P. Márton, and M. Gonçalves, as well as the financial support by the Czech Science Foundation (project no. 19-28594X).

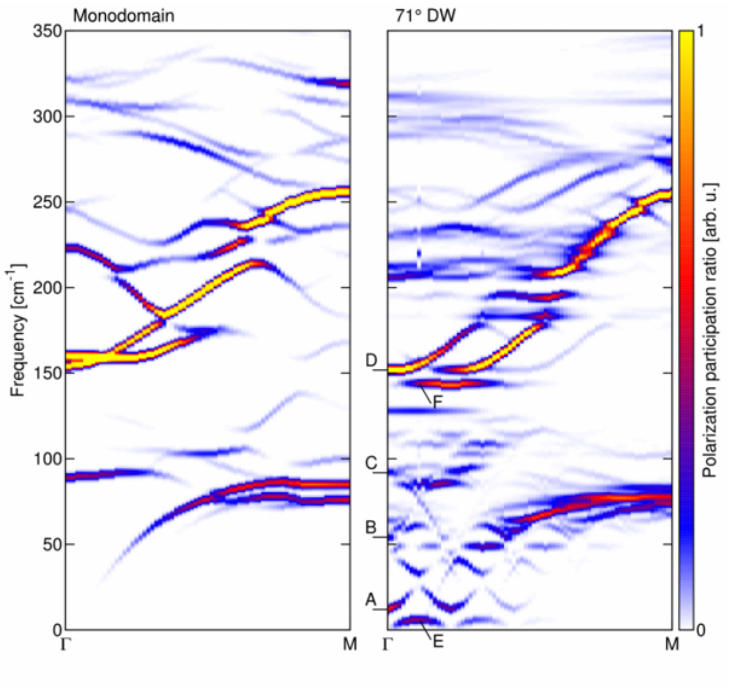

Figure 1: Changes in the phonon spectrum due to presence of a nanoscale domain structure of $BiFeO_3$ (right panel) in comparison with the single-domain case (left panel). It is predicted that the domain-texture related low-frequency Γ-point mode labelled A may lead to a 25-fold enhancement of permittivity when the domains are engineered as just a few nm thick lamellae [3].

[1] J. Hlinka et al., *Terahertz-Range Polar Modes in Domain-Engineered $BiFeO_3$*, Phys. Rev. Lett. **119**, 057604 (2017).

[2] P. Marton et al., *Divergence of dielectric permittivity near phase transition within ferroelectric domain boundaries*, Phase Transitions **86**, 103 (2013).

[3] Q. Li et al., *Subterahertz collective dynamics of polar vortices*, Nature **592**, 376 (2021).

[4] M. Paściak et al., *Dynamics of polar skyrmion bubbles in $PbTiO_3/SrTiO_3$ superlattices*, presentation at this DyProSo symposium.

[5] M. A. P. Gonçalves et al., *Antiskyrmionic ferroelectric medium*, (2023). arXiv:2303.07389

Dynamics of polar skyrmion bubbles in $PbTiO_3/SrTiO_3$ superlattices

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$PbTiO_3/SrTiO_3$ superlattices (PTO/STO) have been recently proving to be a fertile ground for the emergent physical phenomena. Depending on the geometrical constraints and external conditions or stimuli they can host polarization vortex tubes [1], complex domain structures or skyrmion bubbles [2]. Here we extend our previous work on the dynamics of polar vortices in PTO/STO [3] towards the lattice of polar skyrmions. To this end we use shell model and follow two computational strategies for investigating lattice dynamics. By diagonalizing the dynamical matrix of the system of up to 4 skyrmion bubbles we get the full information (eigenvalues, eigenvectors) on harmonic excitations. On the other hand, with molecular dynamics (MD) we treat a larger system at finite temperature. The MD trajectories are then analyzed by inspecting dynamical structure factor $S(q, \omega)$ in important directions in the reciprocal space (see figure below). Combining these approaches allows us to describe the sub-THz optic modes and their interaction with acoustic excitations at small q values.

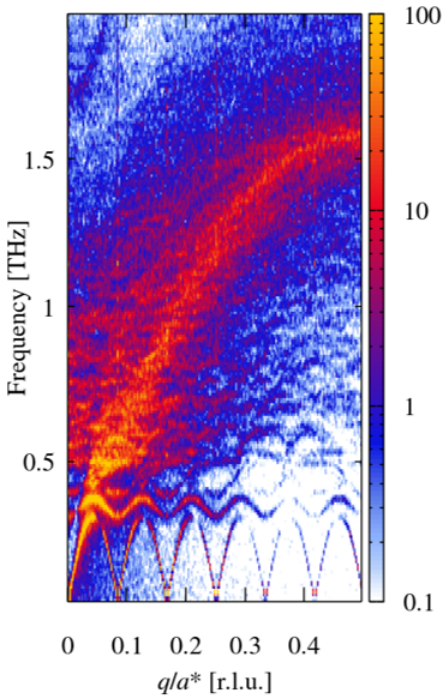

Figure 1: The dispersion curve calculated from molecular dynamics trajectory using program MP_tools [4]. Transverse dispersion along $q80$ direction reveals sub-THz optic modes interacting with the transverse acoustic branch. The lowest-frequency (∼0.3 THz) mode corresponds to the vortexon mode of the vortex-lattice system in PTO layers [3].

[1] A. K. Yadav et al., *Observation of polar vortices in oxide superlattices*, Nature **530**, 198 (2016).

[2] S. Das et al., *Observation of room-temperature polar skyrmions*, Nature **568**, 368 (2017).

[3] Q. Li et al., *Subterahertz collective dynamics of polar vortices*, Nature **592**, 376 (2021).

[4] J. Kulda, https://mptools.fr

New insights into hard antiphase domain boundaries in strontium titanate from Landau-Ginzburg theory and DFT

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Recently [1] the emergence of polarity of so-called hard antiphase boundaries (APBs) in strontium titanate (STO) was investigated using atomistic simulations based on machine-learned force fields. Comparing order parameter (OP) and polarization profiles to those numerically obtained from a standard Landau-Ginzburg-Devonshire (LGD) parametrization produces good agreement of the structural order parameter amplitudes, but fails dramatically in reproducing the domain wall polarization properties. While the atomistic simulations yield a non-zero domain wall polarization up to at least 120 kbar, LGD theory would predict a sharp transition to zero at a pressure as low as 4.6 kbar. A semi-quantitative agreement can be restored by adding so-called rotopolar couplings [2, 3] to the LGD potential and by considering the effects of nuclear quantum fluctuations. Additional evidence for the correctness of our approach is provided by comparing the temperature dependence of the domain wall polarization to recent experimental depolarization pyrocurrent measurements [4]. Our new results [5] illustrate the importance of accounting for nuclear quantum effects beyond standard atomistic approaches in the investigation of domain wall properties.

[1] A. Tröster, C. Verdi, C. Dellago, I. Rychetsky, G. Kresse, and W. Schranz, *Hard antiphase domain boundaries in strontium titanate unravelled using machine-learned force fields*, Phys. Rev. Materials **6**, 094408 (2022).

[2] W. Schranz, C. Schuster, A. Tröster, and I. Rychetsky, *Polarization of domain boundaries in $SrTiO_3$ studied by layer group and order-parameter symmetry*, Phys. Rev. B **102**, 184101 (2020).

[3] A. Schiaffino and M. Stengel, *Macroscopic Polarization from Antiferrodistortive Cycloids in Ferroelastic $SrTiO_3$*, Phys. Rev. Lett. **119**, 137601 (2017).

[4] R. Cabassi, S. Checchia, G. Trevisi, and M. Scavini, *Low temperature ferroelectricity in Strontium Titanate domain walls detected by depolarization pyrocurrents*, Materials Today Communications **28**, 102742 (2021).

[5] A. Tröster, J. Pils, F. Bruckner, C. Verdi, I. Rychetsky, and W. Schranz, *New insights into hard antiphase domain boundaries in strontium titanate from Landau-Ginzburg theory and DFT*, submitted to Phys. Rev. B (2023).

Dielectric properties of Li-doped $KTaO_3$ ceramics compared to crystals

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$K_{1-x}Li_xTaO_3$ ceramics with $x = 0.05$ and 0.1 (KLT5 and KLT10) are prepared by conventional solid-state reaction method and studied in the 15–300 K temperature range using different spectroscopic techniques (resonant microwave, time-domain THz and far-infrared reflectivity) [1]. These data are combined with earlier published dielectric properties in the 100 Hz – 100 MHz frequency range [2]. The broad-band dielectric response of ceramics in the 100 Hz – 20 THz frequency range is compared with that recently published for KLT4.3 and KLT8 crystals [3].

We observe a good qualitative agreement between ceramics and crystals with similar Li-doping in the broad-band dielectric response up to the THz range. In ceramics, the main dielectric relaxation due to the Li^+-ion hopping by $\pi/2$ follows the Arrhenius-type thermal excitation in perfect agreement with that in crystals. We find additional relaxation, which is not thermally activated, and which is not observed in crystals, can be assigned to piezoelectric resonances on the grain boundaries [1]. The coexistence of a relaxor phase with a percolated ferroelectric (FE) phase below the FE transition temperature can be understood by considering the percolative nature of FE transition in crystals [3]. Moreover, the percolation threshold in ceramics could be grain-size dependent. Unlike in crystals, the FE phase transition temperature in both ceramics appears near 100 K, this behavior can be explained by the inhomogeneity of the Li content within individual grains of KLT5.

[1] D. Nuzhnyy, J. Petzelt, V. Bovtun, M. Kempa, D. Repček, A. Tkach, P. M. Vilarinho, and S. Kamba, *High-frequency dielectric properties of $K_{1-x}Li_xTaO_3$ ceramics compared to crystals*, J. Eur. Ceram. Soc. **43**, 5241–5247 (2023).

[2] A. Tkach, A. Almeida, J. A. Moreira, A. Espinha, M. R. Chaves, J. P. de la Cruz, and P. M. Vilarinho, *Lithium-induced dielectric relaxations in potassium tantalate ceramics*, J. Phys. D: Appl. Phys. **44**, 315406–1/7 (2011).

[3] D. Nuzhnyy, V. Bovtun, E. Buixaderas, J. Petzelt, M. Savinov, M. Kempa, M. Paściak, I. Rafalovskyi, V. Chelod Paingad, P. Kužel, S. Kamba, D. Repček, A. Pashkin, V. A. Trepakov, and Z. Trybuła, *Unusual dynamics of the ferroelectric phase transition in $K_{1-x}Li_xTaO_3$ crystals*, Phys. Rev. B **105**, 184103–1/17 (2022).

Thursday, 28$^{\text{th}}$ Sep 2023

Phase-Locked Photon-Electron Interactions in Electron Microscopes

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In this study, we investigate the strong interaction between excitons and photons in thin films of transition metal dichalcogenides, which give rise to propagating exciton polaritons through self-hybridization effects. Additionally, we showcase how cathodoluminescence spectroscopy can be employed to map the extremely short propagation length of self-hybridized exciton polaritons [1]. Furthermore, we explore the intricate interplay between excitons, photons, and plasmons, resulting in the formation of complex composites with fascinating characteristics, including the emergence of flat optical bands [2].

We also present a novel approach to map ultrafast dynamics with electron microscopes [3] (Fig. 1a). Our method involves utilizing cathodoluminescence spectroscopy, where an electron beam sequentially interacts with an electron-driven photon source [4, 5] and the sample. We achieve phase-locked photons that exhibit mutual coherence with the near-field distribution of the fast-moving electrons. We demonstrate the frequency and momentum-dependent correlation between the electron-driven photon source and the radiation from the sample (Fig. 1b and c). This remarkable level of mutual coherence allows us to perform spectral interferometry using an electron microscope.

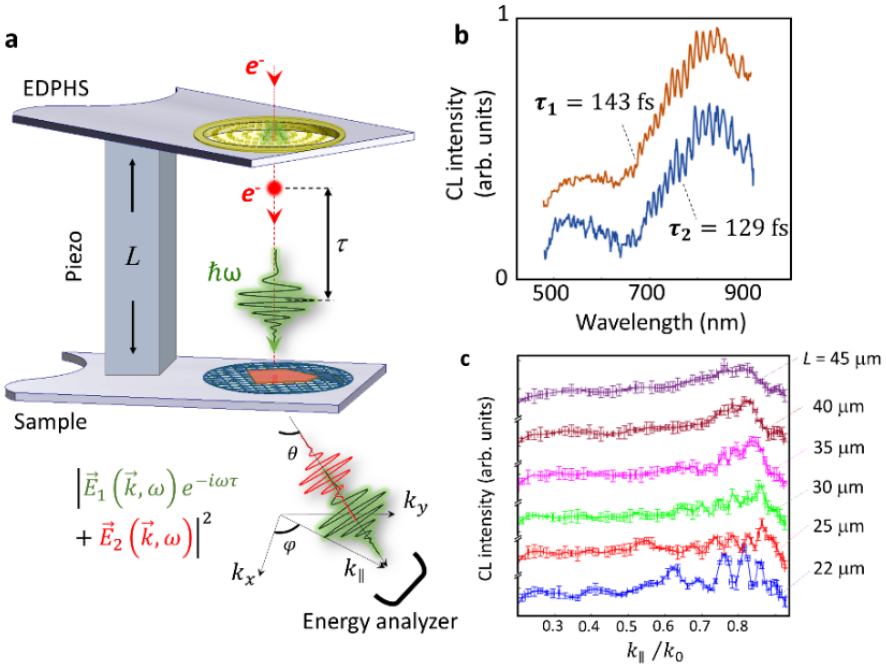

Figure 1: **Performing spectral interferometry with EDPHS in a scanning electron microscope.** (a) Main setup configuration composed of the EDPHS structure and a piezo stage to control the position of the EDPHS structure relative to the sample. A WSe_2 thin flake was used as the sample. (b) Spectral and (c) momentum-space interference fringes at depicted delays/distances between the EDPHS and the sample.

[1] M. Taleb, F. Davoodi, F. K. Diekmann, K. Rossnagel, N. Talebi, *Advanced Photonics Research* **3**, 2100124 (2022).

[2] F. Davoodi, M. Taleb, F. K. Diekmann, T. Coenen, K. Rossnagel, N. Talebi, *ACS Photonics* **9**, 2473–2482 (2022).

[3] M. Taleb, M. Hentschel, K. Rossnagel, H. Giessen, N. Talebi, *Nature Physics* **19**, 869–876 (2023).

[4] N. Talebi, S. Meuret, S. Guo, M. Hentschel, A. Polman, H. Giessen, P. A. van Aken, *Nature Communications* **10**, 599 (2019).

[5] N. van Nielen, M. Hentschel, N. Schilder, H. Giessen, A. Polman, N. Talebi, *Nano Letters* **20**, 5975–5981 (2020).

Induction of electric polarization and magnetization in incipient ferroelectrics by a strong THz electric field

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Juraschek et al. [1, 2] theoretically predicted that circularly polarized phonons should carry orbital magnetic moment even in diamagnetic or paramagnetic materials. The macroscopic orbital magnetic moment should be induced by the excitation of two perpendicularly polarized degenerate polar phonons using circularly polarized THz radiation. Unfortunately, experimental evidence of this phenomenon has been absent until recently [3].

We decided to pump the ferroelectric soft mode in quantum paraelectric $KTaO_3$ single crystal using extremely intense pulses with frequency 0.7 THz. The pulses with a duration of about 10 ps were generated by accelerator-based source with undulator at the TELBE beamline in the Helmholtz Zentrum in Dresden-Rossendorf. The transient magnetic moment on the picosecond time scale was measured via magneto-optic Faraday effect at a probe wavelength of 800 nm. A possible breaking of inversion symmetry was sensed by measuring the second harmonic generation at 400 nm. The experiments were performed between 10 and 300 K.

At low temperatures, the THz pump frequency was close to the soft-mode frequency, and a fairly strong transient birefringence was observed. However, THz pump-induced transient birefringence was detected not only using a circularly polarized THz beam, but also upon pumping with a linearly polarized beam. We explain this by the THz-field-induced ionic electro-optic Kerr effect which was recently observed also in the quantum paraelectric $SrTiO_3$ [4]. In $KTaO_3$, a transient polarization and the related broken inversion symmetry were proved also by measuring the transient second harmonic generation.

Very recently, group of Balatsky theoretically predicted induction of ferroelectric order in quantum paraelectric crystals using off-resonant pumping of the soft optical mode with coherent and linearly polarized THz radiation with suitable polarization [5]. We tried to pump $KTaO_3$ at 20 K with 1.5 and 2.0 THz radiation with different linear polarizations with respect to crystallographic axes, but unfortunately, no second harmonic generation has been detected. Probably much higher amplitude of THz electric field is required.

In summary, we demonstrated that a transient polarization and magnetization can be induced simultaneously, by a strong *resonant* excitation of polar phonons in a diamagnetic and quantum paraelectric crystal $KTaO_3$. A similar effects were recently observed in $SrTiO_3$ [3, 4].

[1] D. M. Juraschek, M. Fechner, et al., *Dynamical multiferroicity*, Phys. Rev. Mater. **1**, 014401 (2017).

[2] D.M. Juraschek, N.A. Spaldin, *Orbital magnetic moments of phonons*, Phys. Rev. Mater. **3**, 064405 (2019).

[3] M. Basini et al., *Terahertz-field driven dynamical multiferroicity in $SrTiO_3$*, arXiv:2210.01690 (2022).

[4] X. Li, T. Qiu, J. Zhang, E. Baldini, J. Lu, A. M. Rappe, and K. A. Nelson, *Terahertz field-induced ferroelectricity in quantum paraelectric $SrTiO_3$*, Science **364**, 1079–1082 (2019).

[5] D. Kuzmanovski, G. Aeppli, et al., *Kapitza stabilization of quantum critical order*, arXiv:2208.09491 (2023).

Pump-probe investigation of spin-lattice coupling in vibronic spin liquid $Tb_2Ti_2O_7$

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Recently, a growing body of work has established the importance of magneto-elastic effects when describing the peculiar magnetic ground-state of the frustrated rare-earth pyrochlore $Tb_2Ti_2O_7$ (TTO) [1–4]. The specific mechanism at play is thought to involve a vibronic hybridisation between the non-Kramers electronic crystal-electric-field levels and the phononic lattice dynamics. The prospect that quantum fluctuations invoked by this spin-lattice coupling could melt the spin-ice properties of TTO is an intriguing possibility.

If correct, this interpretation opens up the potential for exploring new types of spin-liquid behavior driven by hybridized spin-lattice processes. In this context, it is important to have a sound understanding of the principal dynamic processes that occur between the spin and lattice degrees of freedom in TTO. Here, we report on new experimental results involving state-of-the-art pump-probe measurements of TTO, performed at the ELBE free-electron laser in Dresden.

In the experiment, the lattice dynamics are excited with a high intensity 0.7 THz pump pulse while the sample magnetization is monitored by observing the Faraday rotation of an optical probe. The observations (Fig. 1) reveal several intriguing magnetic signatures with different time constants as well as both linear and non-linear responses. The results are discussed in context to the vibronic model which due to a mixing between the global crystal symmetry and the local crystal-field environment predicts a magnetic birefringence.

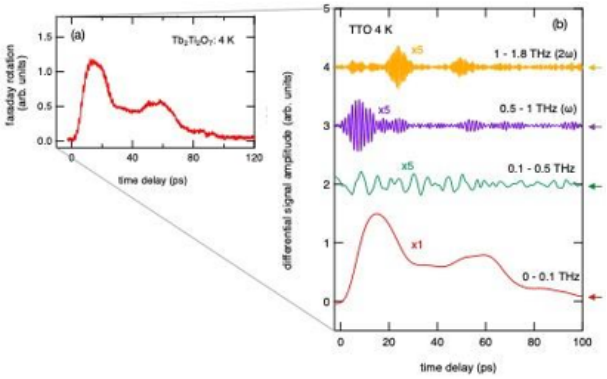

Figure 1: (a) Time resolved Faraday rotation in probe beam after pump pulse. (b) Filtered contributions with different time constants. The purple and yellow curves indicate linear (harmonic) and non-linear (2^{nd} harmonic) responses.

[1] S. Guitteny, J. Robert, P. Bonville, J. Ollivier, C. Decorse, P. Steffens, M. Boehm, H. Mutka, I. Mirebeau, and S. Petit, *Anisotropic Propagating Excitations and Quadrupolar Effects in $Tb_2Ti_2O_7$*, Physical Review Letters **111**, 087201 (2013).

[2] E. Constable, R. Ballou, J. Robert, C. Decorse, J.-B. Brubach, P. Roy, E. Lhotel, L. Del-Rey, V. Simonet, S. Petit, and S. de Brion, *Double vibronic process in the quantum spin ice candidate $Tb_2Ti_2O_7$ revealed by terahertz spectroscopy*, Physical Review B **95**, 020415 (2017).

[3] K. Amelin, Y. Alexanian, U. Nagel, T. Rõõm, J. Robert, J. Debray, V. Simonet, C. Decorse, Z. Wang, R. Ballou, E. Constable, and S. de Brion, *Terahertz magneto-optical investigation of quadrupolar spin-lattice effects in magnetically frustrated $Tb_2Ti_2O_7$*, Physical Review B **102**, 134428 (2020).

[4] Y. Alexanian, J. Robert, V. Simonet, B. Langérôme, J.-B. Brubach, P. Roy, C. Decorse, E. Lhotel, E. Constable, R. Ballou, and S. de Brion, *Vibronic collapse of ordered quadrupolar ice in the pyrochore magnet $Tb_{2+x}Ti_{2-x}O_{7+y}$*, Physical Review B **107**, 224404 (2023).

Magnetic, electric and toroidal order in crystals – $NdFeO_3$ case

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We present [1] the answer to the question: which groups allow to describe a given magnetic, electric and toroidal (anapole) polarization mode? These three classifications are based on magnetic point groups used in two contexts: (i) the magnetic point group of the magnetic crystal class and (ii) the magnetic site symmetry point group of the Wyckoff position of interest. Magnetic, electric and toroidal modes are considered in a restricted sense, i.e. as set-of-directions, disregarding the atomic positions. For magnetic, electric and toroidal orderings there are 64 modes: 3 pure ferro(magnetic/electric/toroidal) modes, 13 mixed ferro(magnetic/ electric/toroidal) with antiferro(magnetic/electric/toroidal) modes, and 48 pure antiferro-(magnetic/electric/toroidal) modes. The proposed classification of modes leads to useful observations: the electric and toroidal modes have many symmetry limitations similar to those already known for the magnetic modes [2, 3], e.g. continuous reorientations of the magnetic or electric or toroidal moments are possible only in triclinic or monoclinic symmetry. Similarly, antiferro(magnetic/electric/toroidal) ordering with a weak perpendicular ferro-(magnetic/ electric/toroidal) component is possible only in monoclinic or orthorhombic symmetry.

To visualize the similarities of magnetic, electric and toroidal modes, we propose a new Rotation-Inversion (RI) notation [1] of magnetic point groups which does not prioritize or distinguish any of three generalized inversions: space inversion, -1, time inversion, 1', and both space-and-time inversion, -1'. Each operation O from a magnetic point group is a product O = RI of one proper rotation R = 1, 2, 3, 4 or 6 and identity or one of generalized inversions I = 1, -1, 1' or -1'. Proper rotations transform magnetic, electric and toroidal polarizations in the same way while inversions in different ways. Starting from the magnetic point group which describes a certain mode of the magnetic moment, we can obtain another magnetic point group which describes the same mode for electric polarization by a specific permutation of generalized inversions which changes -1 to 1' in RI decomposition of each operator of the magnetic point group.

The general classifications of electric, magnetic and toroidal modes are presented for the case of $NdFeO_3$. The predicted monoclinic $NdFeO_3$ symmetry [1, 2] leads to a nontrivial Dirac multipoles motif which could be confirmed using neutron diffraction or resonant x-ray diffraction [4].

[1] P. Fabrykiewicz, R. Przeniosło, I. Sosnowska, *Magnetic, electric and toroidal polarization modes describing the physical properties of crystals. $NdFeO_3$ case*, Acta Cryst. A **79**, 80–94 (2023).

[2] P. Fabrykiewicz, R. Przeniosło, I. Sosnowska, *Magnetic modes compatible with the symmetry of crystals*, Acta Cryst. A **77**, 327–338 (2021).

[3] R. Przeniosło, P. Fabrykiewicz, I. Sosnowska, *Crystal symmetry aspects of materials with magnetic spin reorientation*, Acta Cryst. A **74**, 705–708 (2018).

[4] S.W. Lovesey, *Orthoferrite with a hidden lanthanide magnetic motif: $NdFeO_3$*, Phys. Rev. B **107**, 214426 (2023).

Dynamical Properties of $EuAl_{12}O_{19}$ – a Type I Multiferroic Material

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In magnetism, certain crystal structures may lead to a so-called frustrated magnetic state (i.e. all the magnetic interactions cannot be simultaneously satisfied). This happens e.g. in case of a planar triangular ordering of magnetic ions with antiferromagnetic-like exchange interactions, where many spin configurations have a similar energy. Analogously, a frustrated state may occur when electric dipole moments with tendency to align in an antiparallel way form a triangular lattice.

$EuAl_{12}O_{19}$ has a hexagonal structure [1] combining both magnetic and electric triangular sublattices and thus potentially exhibiting both magnetically and electrically frustrated state. Magnetic triangular sublattice consists of Eu^{2+} ions carrying large spin magnetic moment of 7 μ_B. From our measurements, it follows that a long-range magnetic ordering occurs in $EuAl_{12}O_{19}$ below temperature of 1.3 K. Triangular sublattice composed of AlO_5 bipyramids [1], where Al^{3+} ions are trapped in double-well potential, may also carry electric dipole moments at low temperatures. The expected alignment of the neighbouring off-centered Al^{3+} ions is antipolar, similarly as for isostructural M-hexaferrite $BaFe_{12}O_{19}$ [2].

This contribution is mainly focused on dielectric/spectroscopic response of $EuAl_{12}O_{19}$ single crystal in frequency range from 1 Hz up to tens of THz and low temperatures (2–300 K). Dielectric permittivity shows incipient ferroelectric behaviour at high temperatures, while weak electric polarization ($P_S \sim 0.02\ \mu C/cm^2$) emerges below $T_C = 49.5\ K$. $EuAl_{12}O_{19}$ is thus type I multiferroic. The ferroelectric (FE) phase transition is accompanied by an unusual (see Fig. 1) change of slope in temperature dependence of complex dielectric permittivity. Then it exhibits a distinct maximum (significantly below T_C) whose position is frequency dependent. Moreover, no lattice instability is observed (using IR and THz spectroscopy) in the Brillouin zone center near T_C. All these facts are signs of an improper character of the FE phase transition. The dielectric dispersion is caused by a few thermally activated relaxations (R1 and R2 in Fig. 1). R2 exists below T_C only and may be assigned to a ferroelectric domain wall motion, while R1 exists in the whole temperature range. Frequency of the R1 slows down quickly from THz to Hz range, following the Arrhenius law with possible change of its dynamics at T_C. The microscopic origin of R1 may be related to the structural frustration of the triangular lattice, but this is still being discussed.

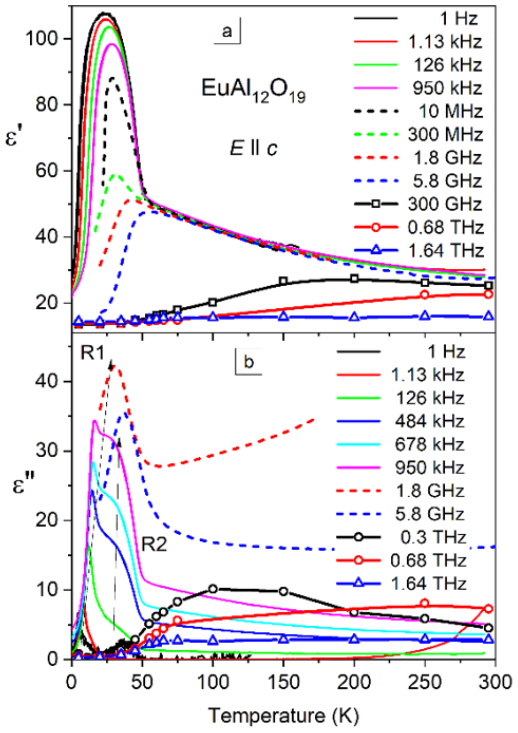

Figure 1: Temperature dependence of real (') and imaginary (") part of permittivity at various frequencies (1 Hz – 1.64 THz).

[1] J.M.P.J. Verstegen, A.L.N. Stevels, *The relation between crystal structure and luminescence in β-alumina and magnetoplumbite phases*, J. Lumin. **9**, 406–414 (1974).
[2] S.P. Shen et al., *Quantum electric-dipole liquid on a triangular lattice*, Nat. Commun. **7**, 10569 (2016).

Spin Waves: versatile, low-dissipation carriers in ferromagnetic systems as a potential source of entanglement

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Spin Waves are the coherent oscillations of the magnetic moments of a medium, they do not involve any charge transfer and hence don't cause Joule dissipation. Even if their fundamental properties are known since decades, their ultimate properties in complex nano-systems are even today a matter of intense investigation both in the theoretical and experimental territories. Their inherent propagation anisotropy is particularly appealing for applications, together with their easy tunability, which comes from Bragg diffraction across the nanostructures and can be controlled by either small magnetic fields or even voltage in multiferroic systems [1]. We review a few spin wave key properties, from a magnetized film, to a lattice of macrospins in an ice-like arrangement (artificial spin ice) and arrays of magnetic vortices. Their intrinsic wave nature, together with the quantization of their energy revealed by light scattering experiments, suggests to realize systems and conditions where spin waves occur as an entangled superposition of otherwise independent states. Following the exposure to tiny magnetic fields or anisotropies introduced in the material by external agents, the superposition breaks down into separate states correlated to the field or anisotropy values [2]. To illustrate the possibility, we discuss spin waves in the vortex state and hybrid spin waves in special ferromagnetic systems, in the perspective of computation and sensing [3].

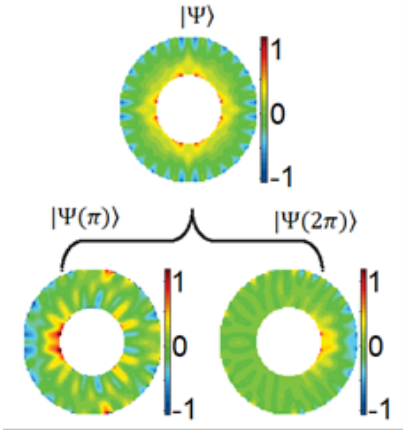

Figure 1: In the case of vortex-magnetization in ferromagnetic rings, the entangled spin-wave state $|\Psi\rangle$ is a radial mode [2], ideally with circular symmetry (fourfold distortion in the figure is due to the square micromagnetic cell used in the simulations). The entangled state is the superposition of two irreducible states $|\Psi(\pi)\rangle$ and $|\Psi(2\pi)\rangle$, which split in the presence of any tiny external magnetic fields or anisotropies.

[1] R. Negrello, F. Montoncello, M. T. Kaffash, M. B. Jungfleisch, and G. Gubbiotti, *APL Mater.* **10**, 091115 (2022).

[2] G. Gubbiotti, M. Madami, S. Tacchi, G. Carlotti, H. Tanigawa, T. Ono, L. Giovannini, F. Montoncello, and F. Nizzoli, *Phys. Rev. Lett.* **97**, 247203 (2006).

[3] Dany Lachance-Quirion, Yutaka Tabuchi, Arnaud Gloppe, Koji Usami, and Yasunobu Nakamura, *Appl. Phys. Express* **12**, 070101 (2019).

Doping and temperature evolution of the electronic properties of electron-doped Sr_2IrO_4 seen by ARPES

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Sr_2IrO_4 is a layered perovskite isostructural to the high T_C cuprate superconductor La_2CuO_4. The strong spin-orbit coupling of the 5d Ir^{4+} ions lifts the degeneracy of the t_{2g} orbitals resulting in a single narrow half-filled band described by pseudospin $J_{eff} = 1/2$ degrees of freedom. This promotes a Mott insulating ground state with antiferromagnetic order below 240 K despite the modest Coulomb interaction in the Ir 5d shell. These similarities with cuprates extend to the unusual metallic state of lightly electron doped Sr_2IrO_4 characterized by Fermi arcs and a pseudogap [1]. Based on this analogy, d-wave superconductivity was predicted [2] but to date no superconductivity was observed down to 100 mK.

In this presentation, I will show Angle Resolved Photoemission (ARPES) results on La doped bulk crystals with higher electron doping than achieved previously (figure 1). Our results show that nodal states become progressively more coherent with increased doping. At the same time, the antinodal pseudogap persists up to the highest doping and up to high temperature, in contrast to previous results on surface doped Sr_2IrO_4 [3].

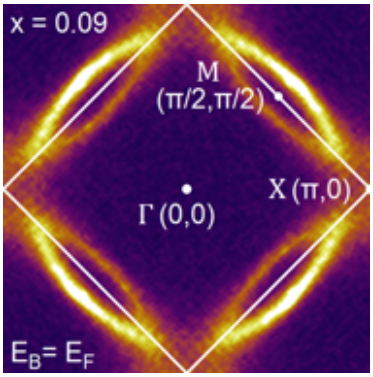

Figure 1: Fermi surface of $(Sr_{1-x}La_x)_2IrO_4$ (x=0.09) showing Fermi arcs along nodal direction and pseudogap along antinodal direction.

[1] A. De La Torre et al., *Collapse of the Mott Gap and Emergence of a Nodal Liquid in Lightly Doped Sr_2IrO_4*, Physical Review Letters **115**, 176402 (2015).

[2] F. Wang and T. Senthil, *Twisted Hubbard Model for Sr_2IrO_4: Magnetism and Possible High Temperature Superconductivity*, Physical Review Letters **106**, 136402 (2011).

[3] Y. K. Kim et al., *Fermi arcs in a doped pseudospin-1/2 Heisenberg antiferromagnet*, Science **345**, 187 (2014).

All optical studies on phonon-magnon coupling in a metallic thin film

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The significant increase in the production of electronic devices and the continuous demand for more efficient, high-capacity, and faster systems have increasingly highlighted the limitations of conventional electronics, fully demonstrating what Moore's law predicted. New fields of exploration have become necessary, and among the most promising is spintronics, where leveraging the quantum property of electron spin could overcome the current limits of electronics. In particular, in recent years, there has been growing interest in the generation and control of spin waves through magneto-acoustic coupling, wherein a surface acoustic wave can guide spin precession [1].

Here we present a four-wave-mixing optical method, called transient grating, for the production and detection of spin waves through the interaction of magnetoelastic coupling [2]. By generating elastic modulation through the interference of two laser pump pulses, we can effectively couple it with the magnetic properties, thus generating a spin wave. By adjusting an external magnetic field applied to thin magnetic films, we can achieve the condition of acoustically-driven ferromagnetic resonance. In this state, the time-varying magnetoelastic field counteracts the Gilbert damping, allowing for an extended duration of spin precession beyond its intrinsic damping.

The combination of a transient grating scheme with time-resolved Faraday polarimetry allows the extraction of the effective magnetization value and the Gilbert damping in nickel thin films [3]. The results are fully consistent with standard FMR measurements.

[1] W. Yang and H. Schmidt, *Acoustic control of magnetism toward energy-efficient applications*, Appl. Phys. Rev. **8**, 021304 (2021).

[2] M. Brioschi et al., *Multidetection scheme for transient-grating-based spectroscopy*, Opt. Lett. **48**, 167 (2023).

[3] P. Carrara et al., *All-Optical Generation and Time-Resolved Polarimetry of Magnetoacoustic Resonances via Transient Grating Spectroscopy*, Phys. Rev. Appl. **18**, 044009 (2022).

Are studies along the elevated pressure pathway providing new knowledge about supercooled liquids' relaxation dynamics? The unique case of some phenyl alcohols.

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For the "high-pressure" community, it is evident that pressure is as significant a parameter as the temperature in studies of the complex properties of various materials in the thermodynamic space. However, this statement remains obscure for many people unfamiliar with high-pressure studies. They still believe that investigations performed only at ambient pressure are sufficient for getting complete knowledge about the features of different materials.

Broadband dielectric spectroscopy is a handy experimental tool for studying dipole glass formers because it enables us to follow their relaxation dynamics over twelve or more decades. And easily detect the differences between various groups of materials.

For example, in the case of compressed *dipropylene glycol* (H-bonded liquid), the structural relaxation broadens compared to the unpressurized sample. In contrast, no broadening is observed for the methylated sample, *dipropylene glycol dimethyl ether* (van der Waals liquid) for different p-T conditions (i.e. so-called time-temperature-pressure superposition is observed) [1]. These differences are related to the existence of supramolecular structures developed via H-bonds. In the case of many monohydroxy alcohols, these structures are chain-like. Their presence is reflected as an additional, exponential process (called *Debye relaxation*), slower than the structural one, more or less visible on the dielectric spectra. It was already shown that increasing pressure modifies these supramolecular structures differently than decreasing temperature. These modifications are observed, as mentioned above, in differences in the relaxation dynamics of the associated material at different thermodynamic paths compared, e.g., for the same time scale of the relaxation processes.

However, for some persons, comparing results for different materials with different values of parameters like viscosity, glass temperature, structural or Debye relaxation times for at least one pair of the same p-T conditions remains unconvincing. They can state that comparisons make sense only if we compare materials with identical properties at the same starting thermodynamic conditions. Usually, it is challenging to find materials that fulfill this criterion. Fortunately, during this presentation, I will show results for phenyl monohydroxy alcohols that exhibit the same temperature behavior of relaxation dynamics at ambient pressure. Only at compression do differences between them become visible. It is a beautiful exemplification of the meaning of high-pressure studies as a necessary tool for understanding the properties of these alcohols in particular and any materials in general.

Acknowledgment: S.P. is thankful for the financial support from the Polish National Science Centre within the OPUS project (no. UMO-2019/35/B/ST3/02670).

[1] K. Grzybowska, S. Pawlus, et al., *Changes of relaxation dynamics of a hydrogen-bonded glass former after removal of the hydrogen bonds*, J. Chem. Phys. **125**, 144507 (2006).

[2] S. Kołodziej, J. Knapik-Kowalczuk, et al., *Essential meaning of high pressure measurements in discerning the properties of monohydroxy alcohols with a single phenyl group*, J. Molecular Liq. **305**, 112863 (2020).

Nonlinear viscoelasticity of tennis balls

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Mechanical properties of sport balls exhibit intriguing kinds of behaviour in spite of being a subject of experimental and theoretical studies for several past decades [1, 2]. Quasistatic compression of 8 tennis balls of different manufacturers and designed for different players, children included, have revealed a power law load-displacement relation in a relatively large range of loads occurring in a real play. Interestingly enough the exponents of the power law are almost universal and close to $6/5 - 4/3$ except for the children ball [3]. This is somewhat different from the findings of [2] for the balls impacting rigid surface. Cyclic compression-release experiments with different displacement rates provide crescent-shaped hysteresis loops hardly reproducible with the simplest viscoelastic models even when a Hookean elasticity is replaced with a power-law [3]. More attempts to determine the nature of the viscoelasticity of the tennis balls, the fractional viscoelasticity included [4] will be presented.

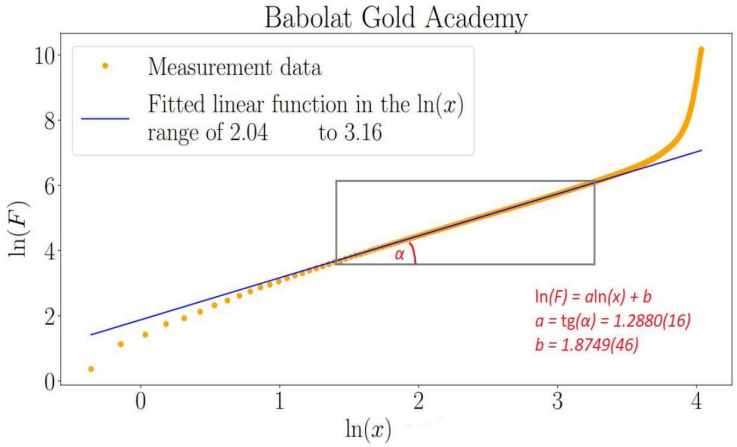

Figure 1: Power law range of force-displacement relation for one of the studied balls.

[1] Lane, B. D., *Advanced techniques to improve the design of tennis ball cores*, Doctoral Thesis, Nanyang Technological University, Singapore (2019).

[2] Goodwill S. R., Haake S. J., *Modelling of tennis ball impacts on a rigid surface*, Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science **218**, 1139–1153 (2004).

[3] Saribekyan, A., *Selected Mechanical Properties of Tennis Balls*, Engineer Thesis, Cracow University of Technology (2023).

[4] Penson K. A., Górska K., Horzela A., *The stretched exponential behavior and its underlying dynamics. The phenomenological approach*, Fractional Calculus and Applied Analysis **20**, 260–283 (2017).

Photostrictive actuators based on freestanding ferroelectric membranes

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Complex oxides offer a range of functional properties and recent advances in fabrication of freestanding membranes of these oxides have enabled enhanced functionality and novel manipulation strategies. We demonstrate photoactuation on freestanding thin film resonators of ferroelectric Barium Titanate ($BaTiO_3$) and paraelectric Strontium Titanate ($SrTiO_3$). The membranes act as nano-drums, oscillating at their natural resonance frequency when illuminated by a frequency-modulated laser. Upon illumination, large out-of-plane deflections develop in $BaTiO_3$ membranes, two orders of magnitude larger than in $SrTiO_3$ ones, providing evidence for a ferroelectric origin of their large photoresponse. Time-resolved X-ray micro-diffraction under illumination and temperature-dependent vibrometry provide combined evidence for a photostrictive strain in $BaTiO_3$ originated from partial screening of polarization by photo-excited carriers. These findings emphasise the pivotal role of light-matter interaction and its manifestation in ferroelectrics such as photostriction, and demonstrate the potential of freestanding ferroelectric membranes as wireless remote optomechanical devices for applications such as photo-actuators and sensors.

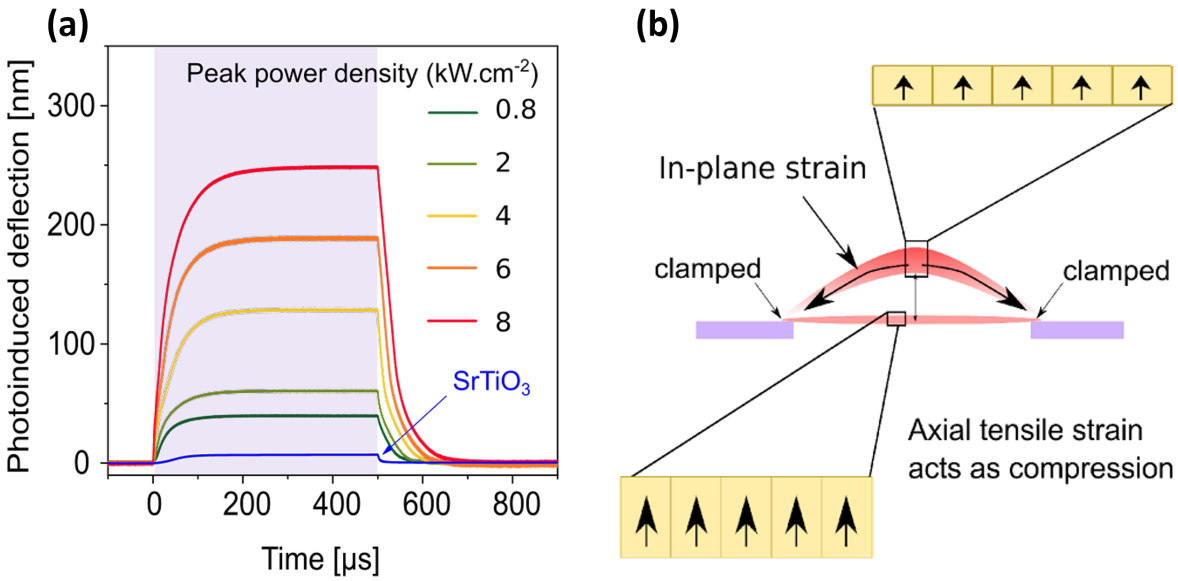

Figure 1: (a) Photoinduced out-of-plane deflection in $BaTiO_3$ & $SrTiO_3$ membranes. (b) Mechanism of photoactuation, originating from photostrictive in-plane strain.

Coupling of multiferroic order parameters in magnetite Fe_3O_4

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Magnetite has long been investigated across many disciplines due to the interplay between it's ferroic order parameters, namely its ferromagnetism, ferroelasticity and ferroelectricity. It is particularly of interest to the multiferroic community for this reason and is the perfect environment to investigate the coupling between its magnetism, spontaneous polarisation and crystal structure.

A host of techniques have been applied to a magnetite single crystal to attempt to begin untangling the interplay between these couplings, such as synchrotron X-ray diffraction, SQUID magnetometry, and various functionalised atomic force microscopies. Particular interest is taken for the material properties across magnetite's Verwey phase transitions at 120 K, where it becomes ferroelastic, and the lower ferroelectric phase transition, which occurs at 38 K.

DYPROSO-2023: SHORT GUIDE (Talks + Posters)

Tuesday 26th September

Welcome

08:45 AM 09:00 AM **Eng**

Keynote I

09:00 AM 10:00 AM **Wosnitza**

10:00 AM 10:30 AM ***COFFEE***

Session 1 (ME)

10:30 AM 11:10 AM **Blackmore**
11:10 AM 11:35 AM **Brioschi**
11:35 AM 12:00 PM **Kuzma**
12:00 PM 12:25 PM **Kamba**

12:30 PM 01:30 PM ***LUNCH***

Session 2 (POSTERS)

01:30 PM 03:00 PM ***POSTERS***

03:00 PM 03:30 PM ***COFFEE***

Session 3 (FE I)

03:30 PM 04:10 PM **Guennou**
04:10 PM 04:35 PM **Milesi-Brault**
04:35 PM 05:00 PM **Goncalves**
05:00 PM 05:25 PM **Ondrejkovic**
05:25 PM 05:50 PM **Zielinski**

06:30 PM *Meeting DyProSo Advisory Board*

Wednesday 27th September

Keynote II

09:00 AM 10:00 AM **Deinert**

10:00 AM 10:30 AM ***COFFEE***

Session 4 (THz I / DS)

10:30 AM 11:10 AM **Kaiser**
11:10 AM 11:35 AM **Adams**
11:35 AM 12:15 PM **Paarmann**
12:15 PM 12:40 PM **Jasiurkowska-Del.**

12:40 PM 01:30 PM ***LUNCH***

Excursion I

01:30 PM 03:30 PM **SLUB / KRO**
[Visits of University Library Treasury and Hermann Krone Collection]

03:30 PM 04:00 PM ***COFFEE***

Session 5 (FE II)

04:00 PM 04:40 PM **Hlinka**
04:40 PM 05:05 AM **Pasciak**
05:05 PM 05:30 PM **Tröster**
05:30 PM 05:55 PM **Nuzhnyy**

07:00 PM ***DINNER***

Thursday 28th September

Keynote III

09:00 AM 10:00 AM **Talebi**

10:00 AM 10:30 AM ***COFFEE***

Session 6 (THz II)

10:30 AM 11:10 AM **Kamba**
11:10 AM 11:35 AM **Constable**
11:35 AM 12:00 PM **Fabrykiewicz**
12:00 PM 12:25 PM **Repcek**

12:30 PM 01:30 PM ***LUNCH***

Session 7 (M)

01:30 PM 02:10 PM **Montoncello**
02:10 PM 02:35 PM **Alexanian**
02:35 PM 03:00 PM **Cucini**

03:00 PM 03:30 PM ***COFFEE***

Session 8 (DS / FE III)

03:30 PM 03:55 PM **Pawlus**
03:55 PM 04:20 PM **Saribekyan**
04:20 PM 04:55 PM **Ganguly**
04:55 PM 05:20 PM **Seddon**

Closing Remarks

05:20 PM 05:30 PM **Eng**