

Microstructure, Magnetic and Electronic Ordering: Interplay and Interactions

784. WE-Heraeus-Seminar

**16 – 19 April 2023
at the Physikzentrum Bad Honnef/Germany**

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Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see <https://www.we-heraeus-stiftung.de>

Aims and scope of the 784. WE-Heraeus-Seminar:

Charge density wave (CDW) phases, also known as Peierls instability, form by non-diffusive structural phase transitions along 1D monoatomic chains, but also in 2D materials. The CDW phase results in a new band structure, comparable to that of a semiconductor, as well as a charge density modulated in real space - i.e. a charge order - which follows this characteristic length. In electrical transport, this results in strongly non-linear I-V characteristics. Incommensurate periodic lattice distortion, the softening of certain phonon modes and Fermi-surface nesting accompanies this phase transition. How does this look in 3D? The most famous example of a non-diffusive structural phase transition in 3D is certainly the martensitic phase transition. Experimental data as well as theoretical work point to similar electronic ordering phenomena in those 3D non-diffusive structural phase transitions. This forms the link to magnetic ordering. The magnetocaloric materials of the first order are characterized by the combination of the magnetic phase transition with the simultaneous change in the lattice structure. The general physical focus is on the analysis of all entropy contributions, e.g. from the lattice transition, the change in magnetization and the contribution of the electrons, in order to understand these results with the underlying microstructural picture of this correlated phase transition. Such investigations can be carried out experimentally in situ in high-resolution state-of-the-art microscopy, providing the input for theory. In this seminar, the fundamental aspects of microstructure, magnetic and electronic ordering: interplay and interactions with regard to phase transitions on the atomic, nano- and microscopic scale are discussed.

The seminar is dedicated to a specialized public and is restricted to 80 participants among which there are around 21 invited speakers, as well as poster presentations. Emphasis is set on giving young investigators at the PhD or PostDoc level the opportunity to participate.

Scientific Organizers:

Prof. Dr. Gabi Schierning

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Introduction

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Registration:

Martina Albert (WE-Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h)
and Monday (08:00 – 12:30 h)

Program

Program

Sunday, 16 April 2023

17:00 – 21:00 Registration

18:00 *BUFFET SUPPER and informal get-together*

Welcome, Evening session

19:30 – 19:40 Gabi Schierning **Common motifs in displacive phase transitions**

19:40 – 19:50 Andreas Hütten **Imaging microstructural impact on magnetic behavior**

19:50 – 20:00 Kai Rosnagel **Notes on charge density waves**

20:00 – 20:45 Anna Böhmer **Electronically driven structural distortion in iron-based superconductors: a model case of nematicity in crystalline solids**

Program

Monday, 17 April 2023

07:30 *BREAKFAST*

Session 1: Microstructures and advanced characterization

08:30 – 09:10 Inga Ennen **Interplay of microstructure and phase transition in shape memory alloys**

09:10 – 09:50 Knut Müller-Caspary **Electrical and structural characterisation of nanostructures by four-dimensional STEM**

09:50 – 10:30 Stephen McVitie **Lorentz transmission electron microscopy investigations chiral synthetic ferromagnetic and antiferromagnet systems**

10:30 – 11:00 *COFFEE BREAK*

Session 2: Ultrafast dynamics

11:00 – 11:40 Claus Ropers **Probing charge-density wave phase transitions and metastable states with ultrafast electron diffraction and microscopy**

11:40 – 12:20 Juras Banys **Microwave and THz characterization of materials**

12:20 – 12:30 **Conference Photo** (in the front of the main entrance)

12:30 *LUNCH*

Program

Monday, 17 April 2023

Session 3: CDW transitions

14:00 – 14:40	Michelle Johannes	The Fermi surface and the CDW phase transition
14:40 – 15:20	Ion Errea	First-principles calculations of charge-density wave transition temperatures: lessons learnt on transition-metal dichalcogenides
15:20 – 16:00	Vladimir Strocov	Materials physics with soft X-Ray ARPES: From bulk materials to heterostructures and impurities
16:00	<i>COFFEE BREAK</i>	
16:00 – 18:00	Poster Session	
19:00	<i>DINNER</i>	

Program

Tuesday, 18 April 2023

07:30 *BREAKFAST*

Session 4: CDW transitions, continued

08:30 – 09:10 David Johnson **Charge density waves, interlayer interactions, and magnetic constituents in designed heterostructures**

09:10 – 09:50 Christopher Renner **Insight into the electronic structure of charge density waves from topographic STM images**

09:50 – 10:30 Jasper van Wezel **Chiral charge ordered domains in 1T-TaS₂**

10:30 – 11:00 *COFFEE BREAK*

Session 5: Ferroelectrics

11:00 – 11:40 Dennis Meier **Emergent functional properties and advanced characterization of ferroelectric domain walls**

11:40 – 12:20 Anna Grünbohm **Interplay of ferroelectric phase transitions domain structure and functional responses**

12:20 *LUNCH*

Program

Tuesday, 18 April 2023

Session 6: Shape memory alloys and multi-caloric materials

- | | | |
|---------------|---|--|
| 14:00 – 14:40 | Jan Frenzel | Electronic and microstructural aspects of NiTi-based shape memory alloys |
| 14:40 – 15:20 | Eckhard Quandt | The role of compatibility in shape-memory oxide ceramics |
| 15:20 – 16:00 | Konstantin Skokov | Dissecting complexity of first-order phase transitions in multi-caloric materials |
| 16:00 | <i>COFFEE BREAK</i> | |
| 16:00 – 17:15 | Poster Session, continued | |
| 17:15 | Appreciation of the WE-Heraeus-Poster awards
About the WE-Heraeus-Foundation | |
| 18:30 | <i>HERAEUS DINNER</i>
(social event with cold & warm buffet with complimentary drinks) | |

Program

Wednesday, 19 April 2023

07:30 *BREAKFAST*

Session 7: Advanced theory

08:30 – 09:10 Frank Lechermann **Metal-to-metal transitions in correlated materials**

09:10 – 09:50 Georg Madsen **Computational phase diagrams with neural-network backed effective harmonic potentials. The case of HfO₂**

09:50 – 10:30 *COFFEE BREAK*

Session 8: Advanced measurement techniques

10:30 – 11:10 Josef Freudenstein **Attosecond shifts in the dynamics of interacting Bloch electrons**

11:10 – 11:50 Toni Helm **High-field superconductivity in UTe₂**

11:50 – 12:00 Gabi Schierner
 Andreas Hütten
 Kai Rosnagel **Closing remarks**

12:15 *LUNCH*

End of the seminar and departure

NO DINNER for participants leaving on Thursday; however, a self-service breakfast will be provided on Thursday morning

Posters

Posters

- | | |
|-----------------------------|---|
| Sergejus Balčiūnas | Dielectric properties of $[\text{NH}_4][\text{Zn}(\text{HCOO})_3]$ metal formate framework doped with alkali metals |
| Laila Bondzio | DSC measurements of shape memory alloys |
| Judith Bünte | Investigation on Magnetic Nanostructures Employing In-Situ TEM-Techniques |
| Thomas Dahm | Change of carrier concentration and energy gain in a CDW phase transition |
| Ralf Drautz | Atomistic modelling of phase transitions with the atomic cluster expansion |
| Ilya Eremin | Collective modes in nonequilibrium dynamics of unconventional superconductors with competing orders |
| Jan Fischer & Daniel Hägele | Microsecond Thermo-Dynamics of ΔT and P in ferroic materials subject to oscillating fields |
| Sven Graus | Influence of external strain on the charge-density wave and superconducting phases of NbSe_2 |
| Markus Gruner | Understanding nanotwinned microstructures in Ni-Mn-based Heusler alloys from first-principles |
| Martin Gutierrez | Purely anharmonic charge-density wave in the 2D Dirac semimetal SnPF |
| Rolf Heid | Soft phonons in CDW phase transitions from first principles |

Posters

Lan-Tien Hsu	Field-Direction-Dependency of the Electrocaloric Effect
Farnaz Kaboudvand	Investigating Electronic Structures of Kagome Metals
Alexander Kunzmann	Single crystal growth of Ni_2MnGa , $\text{Ni}_{48}\text{Co}_5\text{Mn}_{25}\text{Ga}_{22}$ and BaBiO_3
Timo Kuschel	Spin-dependent electron entropy at phase transitions
Johanna Lill	Lattice contribution to entropy change at first order phase transition in Laves phase DyCo_2
Lotte Mertens	Chiral domains in Tantalum disulfide
Martin Mittendorff	Terahertz signatures of the martensitic phase transformation in NiTi alloys
Yousra Ounza	Transport-magnetism correlation in layered perovskite manganite ($\text{LaCaBiMn}_2\text{O}_7$)
Sangeetha N. S.	First-order antiferromagnetic transitions in CaMn_2P_2 and SrMn_2P_2 single crystals containing corrugated-honeycomb Mn sublattices
Lauritz Schnatmann	Investigation of solid-state interface interactions in $\text{FeSe}/\text{TiSe}_2$ multilayers as example for dichalcogenide systems
Chithra Sharma	Addressing the spin-valley flavors in moiré mini-bands of MoS_2
Timon Sieweke	NiTi growth by the micro pulling down method

Posters

Šarūnas Svirskas

**Broadband dielectric spectroscopy of
BaTiO₃-based relaxor ferroelectrics**

Teslin Rose Thomas

**Elastoresistance of the antiferromagnetic
(Ca,Sr)Co₂As₂ system in different
symmetry channels**

Riccardo Vocaturo

**Ab initio DFT investigation of the
inversion-breaking Weyl semimetal PtBi₂**

Abstracts of Lectures

(in alphabetical order)

Microwave and THz characterization of Materials

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The dielectric response of materials provides information about the orientational adjustment of dipoles and the translational adjustment of mobile charges present in a dielectric medium in response to an applied electric field. Microwave and terahertz dielectric spectroscopy of ferroelectrics and related materials enables the independent determination of the dielectric permittivity and loss in the dispersion region, as well as the parameters of the soft modes related to phase transitions.

Besides scientific purposes, microwave dielectric measurements are of increasing importance in telecommunications related applications and the design of microwave circuit components. These applications include imaging radars, guidance systems, surveillance and secure communications. The magnetic properties are also of crucial importance. Dielectric and magnetic parameters fully characterize the manner in which electromagnetic waves propagate within the medium. The difficulties of making measurements on a wide range of materials over a wide frequency (and temperature) range have led to the development of various direct and indirect methods.

At microwave frequencies, the direct single-frequency methods were enriched in the recent years with more convenient broad band frequency domain dielectric spectroscopy (FDDS), time – domain spectroscopy (TDS), Fourier transform spectroscopy (FTS).

Computer controlled spectrometers are now the norm in dielectric spectroscopy. Computers allow the computation of electromagnetic fields in entirely new measurement geometries and the use of numerical analysis in the direct measurement process. The use of such spectrometers is now one of the most fruitful factors in new approaches to microwave dielectric spectroscopy. Each investigator employs the method adequate for the size and shape of a sample. The most important problem now is the rigorous mathematical solution of the microwave interaction with the samples in various geometries.

Although there is now complete overlap and coverage of the radio frequency to the infrared band, the different experimental methods based on coaxial, waveguide, and resonator and free – space technique is still divided and will be presented.

Examples of various ferroelectric, relaxor, dipolar glass materials dielectric spectroscopy results will be presented.

Electronically driven structural distortion in iron-based superconductors: a model case of nematicity in crystalline solids

Anna Böhmer

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Iron-based superconductors are famous for a close interplay of structure, magnetism and superconductivity. A central theme of research is their tetragonal-to-orthorhombic structural transition [1]. There is a consensus that this displacive phase transition is of electronic origin. The corresponding electronic degree of freedom was termed nematic, alluding to the liquid-crystal phase and referring to a lowered rotational symmetry. The nematic degree of freedom seems to derive from stripe-type antiferromagnetism in most - but not all - systems. The existence of an electronic nematic order parameter, irrespective of its microscopic origin, means that there is a related susceptibility. Over the last decade, multiple experimental approaches to the nematic order parameter and nematic susceptibility have been developed. Among other things, they provide experimental evidence for an electronic driving mechanism of the nematic transition.

Nematic transitions have by now been reported in an increasing number of materials, revealing a fascinating richness of phenomenology and mechanism. However, iron-based superconductors remain the ideal systems to study this electronically-driven lattice distortion as its signatures are pronounced, it can be investigated with a wide range of experimental techniques, it is easily tunable, and high-quality single-crystal samples are widely available for these systems [1]. An overview of this “model nematicity” will be given. As a first step towards a wider understanding of nematicity, I will then discuss nematicity in unusual iron- and nickel-based superconductors such as CsFe_2As_2 [2] and $\text{BaNi}_2(\text{As}_{1-x}\text{P}_x)_2$ [3].

References

- [1] Anna E. Böhmer, Jiun-Haw Chu, Samuel Lederer and Ming Yi, *Nature Physics* **18**, 1412 (2022)
- [2] M. Frachet, P. Wiecki, T. Lacmann, S. M. Souliou, K. Willa, C. Meingast, M. Merz, A.-A. Haghighirad, M. Le Tacon and A. E. Böhmer, *npj Quantum Materials* **7**, 115 (2022)
- [3] P. Wiecki, M. Frachet, A. -A. Haghighirad, T. Wolf, C. Meingast, R. Heid and A. E. Böhmer, *Nature Communications* **12**, 4824 (2021)

Interplay of microstructure and phase transition in shape memory alloys

**I. Ennen¹, L. Bondzio¹, J. Bunte¹, D. Stierl¹ D. Ramermann¹
and A. Hütten¹**

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The interplay of microstructure, magnetic and electronic order is a very exciting field that is under continuous research. Especially with regard to phase transitions in shape memory alloys, in order to be able to specifically adjust their properties for applications. For this purpose, modern electron microscopy offers the great possibility to extract information about the atomic structure, chemical nature, magnetic and electrical properties, and their interactions from a sample during the same microscopy session.

Here, we will demonstrate the opportunities in a temperature-dependent manner on a NiCoMnAl magnetic shape memory thin film system as an interesting model system. This Heusler alloys are considered to be promising materials for magnetocaloric cooling applications due to their magnetoelastic coupling near room temperature. Grown in thin film systems of adjacent layers with austenite and martensite crystal structures of almost equal thicknesses, a long range ordering phenomenon in the shape of a 3D checkerboard pattern have been observed in TEM cross section samples [1]. The darker fields of the arrangement consist of martensite nuclei superposed with austenite, while the purely austenite regions appear bright in TEM bright field images. The nucleation process is presumably triggered by inhomogeneous local elastic stray fields of primary martensitic nuclei in the austenite matrix. In order to find limiting parameters of the checkboard pattern formation, the number of the alternating layers as well as the ratio between the thicknesses of the two different layers have been varied. The phase transition has been characterized by temperature dependent TEM analysis. Furthermore, freestanding Heusler films have been prepared and analyzed in comparison to the substrate-bounded systems.

References

- [1] D. Ramermann et al., Applied Sciences **12**, 1748 (2022)

First-principles calculations of charge-density wave transition temperatures: lessons learnt on transition-metal dichalcogenides

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The theoretical ab initio prediction of charge-density wave (CDW) transition temperatures (TCDW) is a complicated task because it requires to include entropic terms in the calculations. In this talk I will show that it is ionic entropy and not electronic entropy which melts the CDW in transition metal dichalcogenides (TMDs). We reach this conclusion by calculating TCDW in bulk and monolayer NbSe₂ [1] fully by first principles within the so-called stochastic self-consistent harmonic approximation (SSCHA) method [2], which can include both ionic and electronic entropy in the calculation of TCDW. The capacity of predicting TCDW's ab initio gives us the opportunity to unveil the origin of the CDW transitions as well as the role that strain, electronic doping, thickness, and van der Waals forces play in the phase transition [3-6].

References

- [1] Raffaello Bianco, Lorenzo Monacelli, Matteo Calandra, Francesco Mauri and Ion Errea. *Physical Review Letters* 125, 106101 (2020).
- [2] Lorenzo Monacelli, Raffaello Bianco, Marco Cherubini, Matteo Calandra, Ion Errea and Francesco Mauri. *Journal of Physics: Condensed Matter* 33, 363001 (2021).
- [3] Raffaello Bianco, Ion Errea, Lorenzo Monacelli, Matteo Calandra and Francesco Mauri. *Nano Letters* 19, 3098 (2019)
- [4] Jianqiang Sky Zhou, Lorenzo Monacelli, Raffaello Bianco, Ion Errea, Francesco Mauri and Matteo Calandra. *Nano Letters* 20, 4809 (2020)
- [5] Jianqiang Sky Zhou, Raffaello Bianco, Lorenzo Monacelli, Ion Errea, Francesco Mauri and Matteo Calandra. *2D Materials* 7, 045032 (2020)
- [6] Josu Diego, A. H. Said, S. K. Mahatha, Raffaello Bianco, Lorenzo Monacelli, Matteo Calandra, Francesco Mauri, K. Rossnagel, Ion Errea and S. Blanco-Canosa. *Nature Communications* 12, 598 (2021).

Electronic and microstructural aspects of NiTi-based shape memory alloys

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NiTi shape memory alloys (SMAs) show fascinating functional properties. They are commercially successful, and they outperform other types of SMAs in terms of mechanical properties, functional stability, corrosion resistance and biocompatibility. The shape memory effect is based on a (almost fully) reversibly martensitic transformation which can be triggered by thermal and mechanical driving forces [1]. Two types of shape memory behavior can be exploited in applications. The thermal shape memory effect (one / two way effect) represents a phenomenon where forward and reverse transformations during cooling and heating result in geometrical changes. In contrast, the mechanical effect (pseudo- / superelasticity) allows the material to tolerate high deformation levels which exceed elastic limits in conventional alloys. The present work gives a brief overview on chemical, electronic, microstructural, and also on engineering / practical aspects of NiTi-based SMAs. It is shown how changes in alloy chemistry affect martensitic transformations [2]. An attempt is made to rationalize compositional effects on the basis of valence electron concentrations. Several examples are presented which document the importance of microstructures, and which demonstrate how dislocations, internal interfaces, and precipitates affect martensitic transformations and thus shape memory effects.

References

- [1] K. Bhattacharya, *Microstructure of Martensite: Why it forms and how it gives rise to the shape-memory effect*, 2004
- [2] J. Frenzel, A. Wiczorek, I. Opahle, B. Maaß, R. Drautz, G. Eggeler, *On the effect of alloy composition on martensite start temperatures and latent heats in Ni-Ti-based shape memory alloys*, *Acta Mater.* **90** 213 (2015)

Attosecond shifts in the dynamics of interacting Bloch electrons

**J. Freudenstein¹, M. Borsch², M. Meierhofer¹, D. Afanasiev¹,
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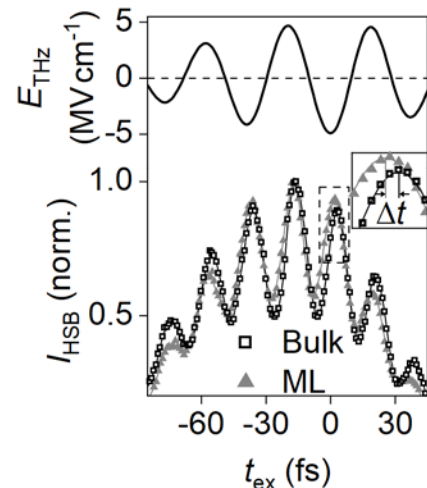
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Correlations between delocalized Bloch electrons are the driving force behind key properties of solids as well as intriguing phase transitions. To directly follow how many-body interactions affect intrinsic electron motion, sub-femtosecond ($1 \text{ fs} = 10^{-15} \text{ s}$) temporal resolution is desirable. Although multi-terahertz (THz) lightwaves have been employed to drive electron currents on subcycle time scales, it has remained an open challenge to resolve the influence of correlations on the trajectories of delocalized Bloch electrons in the time domain.

We will show how many-body correlations modify the dynamics of charge carriers on the attosecond time scale [1]. To this end, coherent excitons are injected in bulk and monolayer (ML) tungsten diselenide (WSe_2) at a precise point in time, t_{ex} . Subsequently, an intense THz light field (Figure, upper panel) accelerates the electron-hole pairs back and forth, resulting in quasiparticle collisions and the emission of light in so-called high-order sidebands (HSB). Crucially, this light is most efficiently generated for specific timing t_{ex} . By comparing the HSB emission from ML (lower panel, triangles) and bulk WSe_2 (squares), attosecond shifts Δt (inset, close-up of the dashed box) with an average value of 1200 as of the optimal injection time become apparent. Due to enhanced excitonic correlations in the ML case, electronic dynamics are altered and thus excitons need to be injected earlier to still enable high-energy recollisions.

Additionally, we observe how increasing the strength of the driving field destroys the excitonic coherence faster and how the valley polarization and Pauli blocking can be exploited to further control the dynamics of charge carriers on the attosecond time scale.

The newly developed attosecond chronoscopy of Bloch electrons could open a new pathway to understanding emergent quantum dynamics and phases.



References

- [1] J. Freudenstein et al., *Nature* **610**, 290-295 (2022)

Interplay of ferroelectric phase transitions domain structure and functional responses

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Not only CDW and magnetocaloric materials but also ferroelectrics show diffusionless phase transitions related to phonon softening and exceptional functional properties. In these insulating materials various competing instabilities and complex phases separated by martensitic transitions can be tuned by composition and elastic boundary conditions.

These transitions are related to enhanced piezoelectric and dielectric responses and allow for a large electrocaloric effect, i.e. adiabatic temperature change in a varying external electrical field, which is promising for novel cooling devices. While ferroelectric phase transitions have been studied for decades and also the understanding of the caloric effect under ideal conditions made important progress in the last years, there are important gaps in knowledge with respect to the electronic and microscopic processes which govern their reversibility, time-stability and tunability [1,2]. Particularly, it is important to understand the impact of the time-dependent microstructure (atomic ordering, defects, domain walls, etc.) on the phase transitions and the functional responses. In this talk I will discuss how ab initio based molecular dynamics simulations allow to isolate these factors and help to predict design rules for ideal microstructures. Thereby I will focus on the coupling between strain, domain structure, and phase transition in prototypical ferroelectric BaTiO₃ [3,4].

References

- [1] A. Grünebohm et al., Energy Technol. **6**, 1491, (2018)
- [2] A. Grünebohm et al, J. Phys.: Condens. Matter **34**, 073002, (2021)
- [3] A. Grünebohm et al, Phys. Rev. Mater. **4**, 114417 (2020)
- [4] A. Everhardt et al, App. Phys. Rev. **7**, 011402 (2020)

High-field superconductivity in UTe_2

**T. Helm^{1,2}, M. Kimata³, K. Sudo³, A. Miyata¹, J. Stirnat^{1,4}, T. Förster¹,
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The heavy-Fermion superconductor UTe_2 is a potential candidate for a spin-triplet superconducting ground state that emerges below 2 K [1,2]. The material is a highly anisotropic paramagnet that exhibits a metamagnetic transition at $H_M = 35$ T for field aligned along the b axis [3]. This transition is associated with a spin reorientation, inducing magnetic fluctuations that may be beneficial for the field-enhanced superconductivity surviving up to H_M . Once the field is tilted away from the b towards the c axis, a reentrant superconducting phase emerges just above $H_M(\theta)$. In addition, field- and pressure-induced superconducting phases with signatures of distinct order parameters have been revealed, adding to the complexity of this material [4,5]. These are only a few of the most recent exciting findings for UTe_2 , leaving many open questions, e.g., about the role of magnetism in the establishment of its unconventional superconducting ground state. In order to better understand the remarkably field-resistant superconductivity we investigated magnetotransport and magnetic torque in pulsed magnetic field up to 70 T for FIB-microfabricated devices. Our findings confirm the existence of the high-field reentrant superconducting phase for a tilt angle around $\theta = 30^\circ$ off the b axis above 40 T. We determined the upper critical field to $H_{c2} \approx 75$ T. Furthermore, the anomalous Hall effect in the normal-state exhibits a drastic suppression in the vicinity of the high-field superconductivity. This new finding calls to revisit the interpretation of the anomalous Hall effect in UTe_2 , and allows a first suggestion of a mechanism for the high-field superconducting phase.

References

- [1] S. Ran et al., *Science* 365, 684 (2019).
- [2] D. Aoki et al., *J. Phys. Soc. Jpn.* 88, 043702 (2019).
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- [4] D. Aoki et al., *J. Phys. Soc. Jpn.* 90, 074705 (2021).
- [5] S. Ran et al., *Nat. Phys.* 15, 1250-1254 (2019)
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The Fermi surface and the CDW phase transition

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Materials properties are determined by both physical and electronic structure and, often, by the interaction of the two. Much of electronic structure boils down to the Fermi surface - a central concept in condensed matter physics and the driving force behind a wide variety of phase transitions and materials behaviors. Instabilities of the Fermi surface are believed to underpin some kinds of magnetism, superconductivity and structural phase transitions such as CDWs. Although the Fermi surface is notoriously hard to measure experimentally, it can be calculated with density functional theory (DFT), opening up the possibility to probe the very basic quantum origins of these novel effects. In this talk, I will argue that, despite the fact that the Fermi surface nearly always gaps as a result of a transition, it is not the whole picture and that states higher and lower in energy (sometimes considerably so) must be considered for a full understanding of how a materials system relieves the burden of high-energy filled states. I will specifically show how the traditional Peierls picture of CDW formation has an extremely limited range of applicability to real systems and demonstrate that electron-phonon coupling is a more relevant mechanism for understanding CDWs and their competitor states: superconductivity and spin-density waves¹.

References

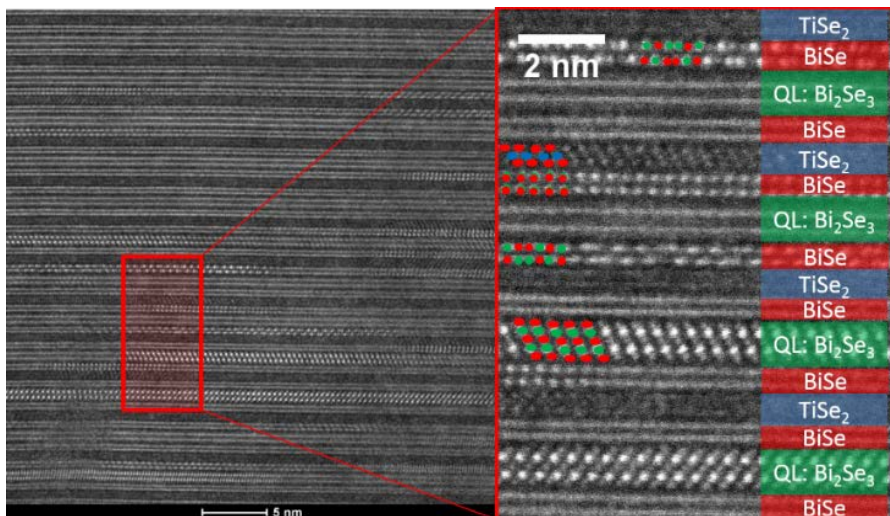
- [1] M. D. Johannes and I. I. Mazin, Phys. Rev. B **77**, 165135 (2008)

Charge density waves, interlayer interactions, and magnetic constituents in designed heterostructures

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Heterostructures consist of two or more compounds with different crystal structures interleaved with targeted constituent layer thicknesses and order. My group has pioneered a synthesis approach based on repeated deposition of a sequence of elemental layers where the number of atoms in each layer correspond to the amount need to form each of the targeted constituent structures. These designed layered precursors self-assemble at low temperatures into the targeted heterostructures because phase segregation into separated bulk constituents is disfavored by low interdiffusion rates. The ability to precisely control constituent layer thicknesses and layer sequences provides opportunities to systematically probe structure-function relationships. We discovered that the charge density wave in $(MSe)_m(VSe_2)_n$ compounds depends on the identity of MSe constituent and the thickness of MSe (m) and VSe_2 (n). We found that the chemical potential difference between constituent layers is compensated by charge donation, leading to systematic changes in electrical transport properties in $[(SnSe)_{1+\delta}]_r[TiSe_2]_q$ heterostructures. We have also discovered that the interaction between constituent layers can stabilize constituent layer structures that are not found as isolated compounds. We have prepared magnetic Pb_2MnSe_3 layers in $(Pb_2MnSe_3)(VSe_2)_n$ heterostructures and a new 1T structured transition metal dichalcogenide, $FeSe_2$, in $(PbSe)_1(FeSe_2)_n$. The ability to prepare families of heterostructures with a variety of constituent layers from designed precursors creates a new "thin film metallurgy" where nanostructure, interfacial phenomena and interlayer interactions can be systematically exploited to manipulate physical properties.



Metal-to-Metal transitions in correlated materials

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The metal-to-insulator transition (MIT) and its associated physics are a hallmark feature of various strongly correlated systems, both on a model-Hamiltonian level as well as concerning real materials. While there are still many open questions regarding such MITs, there is a growing class of materials that show subtle transition characteristics between qualitatively different metallic regimes. For instance, this latter phenomenology has been known already for quite some time in heavy-fermion systems, displaying localized vs. itinerant behavior for f electrons within a sea of other conducting electrons.

In this talk, it will be shown from assessments using first-principles many-body theory by means of the combination of density functional theory (DFT) and dynamical mean-field theory (DMFT), that such metal-to-metal transitions (MMT)s also occur in d electron materials. And also there, these transitions are usually accompanied by rich additional physics. Two examples will be discussed more concretely. First, the MMT in the delafossite compound AgNiO_2 [1,2], involving a distinct structural component to the problem, will be illuminated. Second, the recent theoretical findings of an orbital-selective Mott transition in the van der Waals ferromagnet $\text{Fe}_{3-x}\text{GeTe}_2$ [3] will be discussed. Conclusions on general driving forces for MMTs in d electron materials will be made.

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Computational phase diagrams with neural-network backed effective harmonic potentials. The case of HfO₂

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Methodological advances achieved in the past decades have made it possible to treat temperature-dependent effects within DFT. Arguably the most widespread method is the harmonic approximation (HA), where the displacement-force relationship of the individual atoms is modelled by a harmonic potential. The nuclear Hamiltonian then consists of independent quantum harmonic oscillators which yield an expression for the temperature-dependent free energy. However, for systems unstable at 0 K, in particular those stabilized by temperature, the HA is not applicable. A solution is offered by the effective harmonic potentials (EHPs),[1] which, in essence, involves determining the best HA for the dominating part of the potential energy surface (PES) at a given temperature.

Here, we first describe the temperature-dependent behavior of cubic HfO₂. [2] For this high-symmetry structure, investigation by a DFT-backed EHP approach is made possible by including a reweighting procedure. The reweighting allows direct evaluation of the term responsible for describing anharmonicity in the EHP formalism, as well as the use of unregularized regression techniques.

The EHP relies on importance sampling of the potential energy surface (PES) and for the lower-symmetry monoclinic (*m*) and tetragonal (*t*) HfO₂ phases, a DFT-backed approach incurs an unfeasible computational cost. On the other hand, recent advances in machine learning provide access to exceptionally accurate surrogate PESs. We show how a neural-network force field (NNFF) provides accuracy comparable to DFT at a fraction of the cost.[3,4] We detail data acquisition and training strategies for the low symmetry HfO₂ phases and show how the NNFF-backed EHP gives temperature dependent lattice constants of the *m*- and *t*-phases in excellent agreement with experimental data.[5] In contrast lattice constants substantially lower than experiment are obtained for the studied cubic phases. Furthermore, a *m-t* phase transition temperature is obtained in good agreement with experiment, whereas no cubic phase is found to be stable in the studied temperature range. It is hypothesized that cubic HfO₂ is present only in a defect-stabilized form.

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Lorentz Transmission Electron Microscopy Investigations Chiral Synthetic Ferromagnetic and Antiferromagnet Systems

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Chiral magnetic textures in perpendicularly magnetised magnetic multilayer system have attracted significant interest recently. Such systems incorporating synthetic ferro/ferri/antiferromagnets offer promising applications in the areas of spintronic devices. A wide variety of magnetic textures have been observed from maze like domain patterns as well as skyrmions. Exploring the landscape of these phases including co-existence and control of skyrmion nucleation can be observed using Lorentz transmission electron microscopy. Samples are sputter deposited on thin membranes substrates for TEM observations. Results will be presented for a ferromagnetic coupled film system skyrmions are nucleated at predefined defect sites using focused ion beam microscopy in an applied magnetic field [1]. We also look at antiferromagnetically coupled layers where rich textures have been seen in the transition between AF and FM coupled states. The work presented provides information on plan view and cross-sectional samples in terms of physical, chemical and magnetic structure. Additional metrology is provided VSN-SQUID as well as imaging with large facility beamline experiments.

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Emergent functional properties and advanced characterization of ferroelectric domain walls

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Oxide materials exhibit a broad range of tunable phenomena, including magnetism, multiferroicity, and superconductivity. Oxide interfaces are particularly intriguing. Their low local symmetry combined with the sensitivity to electrostatics and strain leads to unusual emergent phenomena. Recently, ferroelectric domain walls have attracted broad attention as a novel type of oxide interface; the walls are spatially mobile and allow controlling electronic signals at the atomic scale, holding great potential as multifunctional 2D systems. [1]

In my talk, I will present unique features that arise at improper ferroelectric domain walls in different model materials and discuss how these walls can be used to emulate the behavior of key electronic components. To study the domain walls across all relevant length scales down to the level of individual atoms, we apply state-of-the-art microscopy techniques, including 3D imaging by FIB-SEM and atom probe tomography.[2,3] Our work provides new insight into the electronic behavior of ferroelectric domain walls and their interaction with point defects, which is essential to understand their nanoscale physics and ultimately develop them into devices for future nanotechnology.

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Electrical and structural characterisation of nanostructures by four-dimensional STEM

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In recent years, the dimensionality in transmission electron microscopy (TEM) has increased rapidly by the advent of ultrafast cameras that record at frame rates of many kHz. This development has especially paved the way for a revolution as to the versatility of scanning TEM (STEM). In particular, momentum-resolved STEM enhanced traditional Z- and phase-contrast techniques such that any conventional imaging mode is present simultaneously in a 4D data set. Most importantly, the combination of real- and reciprocal space information nowadays allows to quantify charge densities with subatomic resolution¹, to measure polarisation-induced electric fields, and to solve the phase problem by ptychographic techniques.

This presentation includes a brief review of quantitative STEM, followed by selected works on ultrafast detectors. We demonstrate the capability of 4D-STEM using several examples in the field of physical and materials science: First, the concept of first moment imaging is introduced, and its application to the mapping of atomic electric fields in 2D materials is demonstrated². Second, the capability of electrical characterization is expanded to polarisation mapping in semiconductors, where a GaN/AlN system is considered³. Importantly, systematic errors arising from multiple scattering of electrons in the specimen are worked out in detail, and their impact on field mapping in ferroelectrics is shown⁴. Third, a simulation study on the impact of stray fields in electrically contacted specimens for in-situ biasing is reported, with focus the quantitative interpretation of long-range stray fields outside a specimen, in combination with polarisation-induced electric fields inside the material of interest. Forth, a compact prospect will be given as to solving the inverse problem in the presence of multiple scattering based on 4D STEM to retrieve structural details, e.g., ferroelectric ionic displacements in PbZrTiO₃.

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The Role of Compatibility in Shape-Memory Oxide Ceramics

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The systematic tuning of crystal lattice parameters to achieve improved kinematic compatibility between different phases is a broadly effective strategy for improving the reversibility, and lowering the hysteresis, of solid–solid phase transformations. Kinematic compatibility refers to the fitting together of the phases. Here an apparently paradoxical example is presented in which tuning to near perfect kinematic compatibility results in an unusually high degree of irreversibility. Specifically, when cooling the kinematically compatible ceramic $(\text{Zr/Hf})\text{O}_2(\text{YNb})\text{O}_4$ through its tetragonal-to-monoclinic phase transformation, the polycrystal slowly and steadily falls apart at its grain boundaries (a process which is termed weeping) or even explosively disintegrates. If instead the lattice parameters are tuned to satisfy a stronger ‘equidistance’ condition, the resulting material exhibits reversible behavior with low hysteresis. These results show that a diversity of behaviors—from reversible at one extreme to explosive at the other—is possible in a chemically homogeneous ceramic system by manipulating conditions of compatibility in unexpected ways. These concepts could prove critical in the current search for a shape-memory oxide ceramic [1].

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Insight into the electronic structure of charge density waves from topographic STM images

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Charge density waves (CDWs) are the subject of renewed interest to understand their structure, their formation mechanism and their interplay with other quantum phases such as superconductivity and magnetism. Many models have been developed over the years, but they often fail to fully describe specific experimental data sets. Scanning tunneling microscopy (STM) is a prime technique to investigate the CDW ground state. However, the correct identification of the CDW gap in tunneling conductance spectra is highly controversial, as evidenced by the large spread in reported gap amplitudes. Moreover, not all periodic charge modulations observed by STM are CDWs. We will discuss detailed analysis of the CDW modulation amplitudes and phases in topographic images [1], with unprecedented insight into the CDW gap [2], including evidence for its multiband nature [3]. We find compelling evidence that the CDW gap can open significantly below the Fermi level [2] and shift as a function of the local carrier concentration [4]. The latter provides an alternative view on the competition between the CDW and superconducting ground states. Finally, we show that the periodic structures observed in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ lack characteristic features expected for a CDW, thus questioning the existence of a CDW in several high temperature superconductors.

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Probing charge-density wave phase transitions and metastable states with ultrafast electron diffraction and microscopy

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Active optical control of materials promises novel functional states and devices. In recent years, there has been considerable interest in using light to manipulate electronic phases, charge ordering, and interlayer correlations in low-dimensional materials. These approaches promise ultrafast, reversible, and non-invasive control of properties. In this context, we study mechanisms of light-induced phase transitions by developing ultrafast imaging and diffraction techniques.

We recently investigated the coherent control over metal-to-insulator transitions in low-dimensional systems, which are important for their ultrafast changes to electronic and lattice properties. In particular, we demonstrated the role of vibrational coherence in controlling a metal-insulator structural phase transition in a quasi-one-dimensional solid-state surface system [1]. Utilizing double-pulse excitation to switch the system to a metastable metallic state, delay-dependent oscillations of the relevant collective amplitude modes indicate a ballistic component of the transition.

Using Ultrafast Transmission Electron Microscopy (UTEM), we track the evolution of the order parameter in charge-density wave (CDW) domains of 1T-TaS₂ with simultaneous femtosecond temporal and nanometer spatial resolution. Specifically, a tailored dark-field scheme allows for the observation of relaxation pathways and the dynamics of phase boundaries [2]. Tilt-series ultrafast nanobeam electron diffraction in the transformed regions reveals an intermittent suppression of out-of-plane structural correlations. This dimensional crossover coincides with a loss of in-plane translational order, suggesting the formation of a transient hexatic state [3].

Finally, recent single-pulse quench experiments on the low-temperature commensurate CDW phase in 1T-TaS₂ will be discussed, revealing the coexistence of opposing chirality as a structural characteristic of the light-induced hidden states [4].

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Dissecting complexity of first-order phase transitions in multi-caloric materials.

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Materials with a first-order phase transition are of great interest for emerging alternative solid-state refrigeration technologies. For these materials, an application of the different generalized thermodynamic forces/fields is accompanied by large discontinuities and abrupt changes in their conjugate variables, resulting in a large caloric effect. For the rational design of these materials, it is vitally important to know in detail, how different subsystems of the solid interplay during the transition, which system triggers the phase transformation, and how this mutual entanglement interaction can be responsible for the resulting thermal effects.

In this talk, we will discuss a new pathway to disentangle the interplay between the structural, magnetic and electronic degrees of freedom. We believe that our approach serves as the next step towards a complete understanding of the driving forces of the transition, together with comprehension of the origin of thermal hysteresis in magnetic phase-change materials [1]. Recently, we have built several original experimental setups for simultaneous measurement of macroscopic physical properties (magnetization, magnetostriction, resistivity, temperature change) in isothermal or adiabatic conditions [2], [3]. These devices were used for study materials with first-order magneto-structural phase transition, such as La(Fe,Si)₁₃, Heusler alloy, FeRh and RCo₂. The elastic and magnetoelastic coupling constants were quantified, which in turn allowed us a better understanding of the intriguing nature of the phase transitions caused by the magnetic field change and stress.

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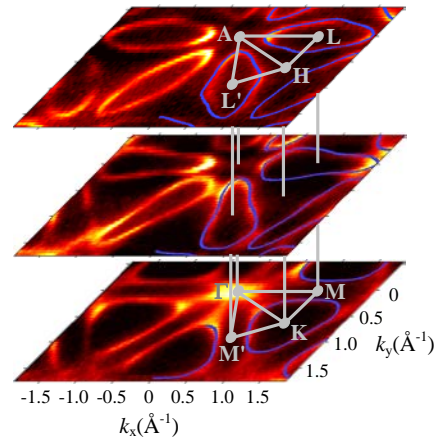
Materials Physics with Soft X-Ray ARPES: From Bulk Materials to Heterostructures and Impurities

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Soft-X-ray ARPES in the photon energy range around 1 keV enhances the \mathbf{k} -resolving capabilities of this experimental technique with large probing depth and resonant photoexcitation delivering chemical specificity. These advantages allow access to 3D bulk materials, buried heterostructures and impurity systems for real electronic devices.

Bulk materials. – Applications of soft-X-ray ARPES to 3D bulk materials are based on sharp definition of the out-of-plane \mathbf{k} resulting from the enhanced photoelectron delocalization. This is illustrated, for example, by the Fermi surface of VSe_2 measured at $h\nu$ around 1 keV (Figure). Its autocorrelation analysis reveals an out-of-plane nesting which acts as the precursor for the exotic 3D charge density waves [1]. Further examples include 3D band dispersions in topological materials, quasicrystals, \mathbf{k} -dependent electron-phonon interaction in complex oxides [2], etc.



Buried heterostructures. – Semiconductor systems are illustrated by AlN/GaN high-electron-mobility transistor (HEMT) heterostructures, where soft-X-ray ARPES resolves the anisotropic Fermi surface (Figure) and band dispersions of the interfacial quantum-well states [3]. A paradigm example of oxide interfaces is $LaAlO_3/SrTiO_3$. Resonant photoexcitation at the Ti L -edge resolves here the interfacial states, whose peak-dip-hump spectral function identifies their multiphonon polaronic nature [4].

Impurity systems. – An example of impurity systems is Ga(Mn)As where resonant photoexcitation at the Mn L -edge identifies the energy alignment and hybridization of the Mn impurities with host GaAs, disclosing the mechanisms of the ferromagnetic electron transport [5].

Finally, I introduce an ongoing instrumental project on iMott the multichannel spin detector that boosts the spin detection efficiency by a few orders of magnitude, allowing access to spin textures of heterostructure and impurity systems for spintronics.

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Chiral charge ordered domains in $1T\text{-TaS}_2$

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Recent scanning tunnelling microscopy experiments of the nearly commensurate charge density wave (CDW) in $1T\text{-TaS}_2$ reveal a continuous evolution of the CDW lattice from domain wall to domain centre, instead of a fixed CDW arrangement within the domain. Furthermore, it is found that an intra-domain chirality characterises the nearly commensurate phase [1]. Unlike the orbital-driven chirality previously observed in $1T\text{-TiSe}_2$ [2], the chiral nature of the domains in $1T\text{-TaS}_2$ appear to be driven by strong coupling of the CDW to the atomic lattice [1]. We will present a macroscopic order parameter theory describing the emergent chirality, and discuss its implications for $1T\text{-TaS}_2$ and other transition metal dichalcogenides.

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Abstracts of Posters

(in alphabetical order)

Dielectric properties of $[\text{NH}_4][\text{Zn}(\text{HCOO})_3]$ metal formate framework doped with alkali metals

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Recently a metal organic framework $[\text{NH}_4][\text{Zn}(\text{HCOO})_3]$ has attracted interest of the scientific community. According to Guan-Cheng Xu et al. a paraelectric – ferroelectric phase transition (from $P6_322$ to $P6_3$) was reported at 181 K temperature [1]. Furthermore, MOFs are likely candidates for magnetism, due to possibility to change metal centers, thus having a potential for single crystal multiferroic materials. Our initial studies revealed a tendency of alkali metals to diffuse into the structure of $[\text{NH}_4][\text{Zn}(\text{HCOO})_3]$. Hence, the aim of this work is to investigate the effect on dielectric properties of K impurities in the $[\text{NH}_4][\text{Zn}(\text{HCOO})_3]$ crystal structure.

Dielectric measurements were performed in 130 – 300 K and 10 Hz – 1 GHz frequency range using HP 4284A LCR meter and Agilent 8714ET vector network analyzer. The crystals were cut in such a way that during electrical measurements the field in the crystal was parallel to the z axis. Experiments were performed at 1 K/min cooling/heating rates. Initial study show a slight shift of paraelectric – ferroelectric phase transition temperatures from 180 K to 161 K. Furthermore result show a clear relaxation below phase transition temperature which can be linked to domain wall motion. Lastly experimental data was approximated using superposition of several Cole – Cole functions. Obtained relaxation time were further approximated using Arrhenius law. Calculated activation energies for low temperature relaxation are $E_A=0.15 \pm 0.02$ eV for pure and $E_A=0.34 \pm 0.02$ eV for sample with 5% potassium impurities. Significant increase in activation energies could have occurred due to domain wall pinning to point defects, caused by potassium, which would hinder domain wall motion

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DSC measurements of shape memory alloys

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For the investigation of phase transition effects in shape memory alloys it is useful to predetermine the transition temperature range and entropy of the system. Therefore differential scanning calorimetry (DSC) measurements are essential.

Even small changes in the composition of shape memory alloys may have major impact on the transition temperature as it can be seen in DSC measurements for NiTi alloys.

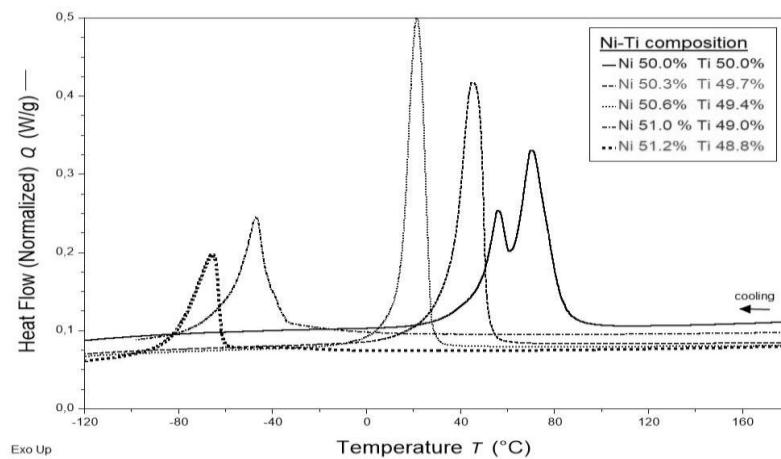


Fig.1: Austenite to Martensite transition for different NiTi-alloys

Commonly bulk or powder samples of at least few mg are used for DSC measurements, but testing the lower weight limits of the DSC 25 device has shown, that calorimetric effects in samples with very low weight such as below 1mg can be seen.

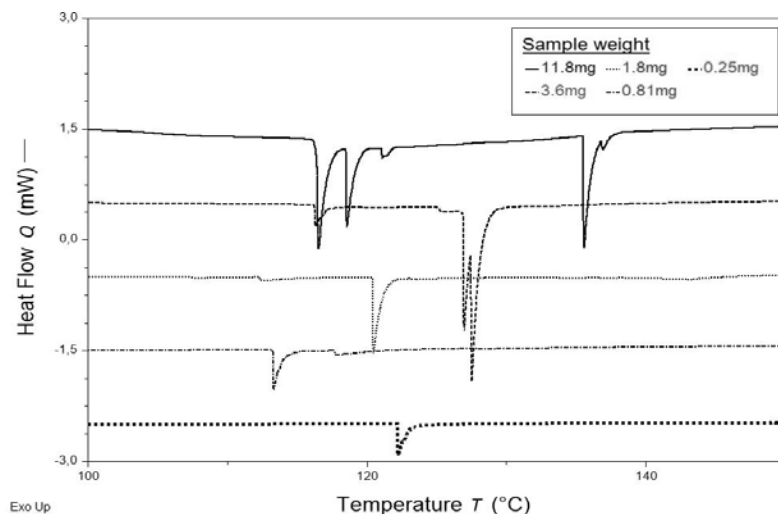


Fig.2: Calorimetric effect for different masses of NiCoMnGa with an offset in Q

Investigation on Magnetic Nanostructures Employing In-Situ TEM-Techniques

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The invention of Transmission Electron Microscopy (TEM) in 1931 by Ernst Ruska and Max Knoll gave solid state physics a more detailed insight into the structure of crystals. In this type of microscopy, the complete sample is traversed by the electrons. The structure of the solid has an influence on the deflection of the electrons, but also the electric and magnetic fields inside the sample. This additional deflection is described by the Lorentz force. Magnetic microscopy allows the user to determine information about the magnetic conditions of the sample.

Two different types of magnetic microscopy are used here: Differential Phase Contrast (DPC) and Lorentz microscopy. While DPC requires a separate segmented detector, Lorentz microscopy can be conducted with a conventional detector.

To deflect the electron beam, an in-plane field component is needed. To induce such an in-plane component in the sample, it is tilted to $\pm 25^\circ$ in the TEM and magnetized through the objective lens. The objective lens is controlled separately by the user, who, through changing the settings of the objective lens, can change the appearing field. Setting different magnetic fields allows to investigate the influence of the magnetic field on the sample.

In addition to the before mentioned magnetic field, the user can heat the sample with a specimen heating holder. This enables the investigation of a temperature dependent magnetic condition.

Overall, these two in-situ TEM techniques allow the characterization of the magnetic behaviour of samples under different constraints.

To show the heating toolchain, a cobalt thin film is investigated in a temperature range from room temperature to 600 °C. The magnetic nanostructure of the sample after heating is imaged. This sample is again heated up and the domain wall width in dependence of the temperature is measured. This series is investigated in Lorentz microscopy.

Furthermore, the influence of the magnetic field is investigated in a nanostructured GMR stack. This allows us to investigate the remagnetization of single domains inside the structure. This sample is investigated with DPC.

Change of carrier concentration and energy gain in a CDW phase transition

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Recent experimental studies of electrical and thermal transport in the shape memory alloy NiTi found large changes in the carrier concentration and their mobility [1]. The electronic contribution to the total entropy at the phase transition was found to be surprisingly high, of the order of 30%, which suggests an important contribution of the conduction electrons to the martensitic phase transition. These results have been interpreted in terms of the formation of a charge density wave (CDW). Here, we investigate a simple tight-binding model for the formation of a CDW. We calculate the change in carrier concentration and energy gain of the electrons. The results are compared with the experimental findings on NiTi.

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Atomistic modelling of phase transitions with the atomic cluster expansion

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Modelling phase transitions atomistically is a difficult challenge. On the one hand one needs fast and efficient interatomic interaction models that enable millions or billions of force and energy evaluations to be carried out, as required for predicting free energies and related thermodynamic properties. On the other hand, the interatomic potentials must be accurate and transferable to provide reliable estimates of the free energies of competing phases.

In the past 15 years machine learning interatomic potentials became available that can represent energies and forces from density functional theory calculations accurately and therefore enable the simulation of phase diagrams. I will focus on the atomic cluster expansion (ACE) [1] for modelling the interatomic interaction. To this end I will discuss the implementation [2] and parameterization [3] of ACE including active learning strategies [4]. I will then show applications of ACE to computing structural stabilities, defects and phase transitions in carbon, magnesium, Ni-Ti, Pt-Rh and water.

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Collective modes in nonequilibrium dynamics of unconventional superconductors with competing orders

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The recent technological development of THz spectroscopy makes it possible to probe properties of quantum matter, which cannot be observed in equilibrium. This is of considerable interest in the field of unconventional superconductivity, where controlled probing of the relaxation dynamics yields access to understanding ground state properties of the underlying system and access the competing orders.

Motivated by the recent development of terahertz pump-probe experiments, we will discuss the short-time dynamics in superconductors with multiple attractive pairing channels and competing instabilities. Studying a single-band and multiband superconductors, we analyze the signatures of collective excitations of the pairing symmetries (known as Bardasis-Schrieffer modes) as well as the order parameter amplitude (Higgs mode) in the short-time dynamics of the spectral gap and quasiparticle distribution after an excitation by a pump pulse. We show that the polarization and intensity of the pulse can be used to control the symmetry of the non-equilibrium state as well as frequencies and relative intensities of the contributions of different collective modes[1-2].

Finally, I address the question of whether pump-probe technique can be used to reveal an interplay between various collective modes visible in the superconducting state and to distinguish the Pomeranchuk nematic collective mode from the BS mode due to the subdominant Cooper-pairing channel[3-4].

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Microsecond Thermo-Dynamics of ΔT and P in ferroic materials subject to oscillating fields

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The thermodynamic response of many materials to a changing external parameter exhibits often a peculiar frequency dependence. Frequency dependent polarization-loops, $P(E)$, or magnetization-loops, $M(H)$, are found in many ferroelectrics (like BaTiO₃) or metamagnets (like LaFeCo). We argue that a time-resolved study of the field-induced (adiabatic) temperature change ΔT in addition to P or M gives a much more comprehensive understanding of the truly *thermo-dynamical* behavior of materials.

Here, we present the dynamical $\Delta T(t)$ of the electrocaloric effect in BaTiO₃ with mK temperature resolution and μ s temporal resolution in an oscillating electric field. Temperature data are obtained under close-to-adiabatic conditions via infrared emission [1,2]. An almost parabolic dependence of ΔT on E is found below $f = 2.7$ Hz. At increasing frequencies, a phase shift of several degrees between ΔT and E becomes apparent and an additional asymmetry of ΔT regarding the sign of E occurs which is not found in simultaneously measured $P(E)$ loops. We guess that the former effect may be due to a close-to-resonance piezoelectric deformation of the sample which creates a phase shifted contribution to ΔT . The latter effect may be due to a built-in static polarization. We also show magneto-caloric measurements in LaFeCoSi at its Curie-temperature where we find negative plateaus in the cyclic $\Delta T(t)$ whose temporal widths increase with frequency. In contrast, no plateaus are found in Gd. Latent heat diffusion may strongly influence the field induced PM to FM transition at phase boundaries. Our non-standard ΔT -measurements highlight that microstructure can strongly influence thermo-dynamic behavior. Time-resolved strain-measurements and optical soft-mode spectroscopy will be discussed as possible future methods for gaining a more comprehensive picture of *thermo-dynamics*.

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Influence of external strain on the charge-density wave and superconducting phases of NbSe₂

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Hexagonal 2H-NbSe₂ is a quasi-two-dimensional material known for the co-existence of superconductivity below 7.8 K and a charge-density wave (CDW) phase below 34 K. Recently, theoretical studies investigated the relation between these two phases, suggesting a highly anisotropic superconducting gap [1]. Over the past few years, strain has come into focus as a parameter to control and study quantum materials. For example, the elastoresistance, i.e., the strain-dependence of the electrical resistance, is intensely investigated in the context of nematic materials [2] and large uniaxial strain was used to stabilize an otherwise elusive CDW in a cuprate superconductor [3].

We have synthesized thick and mm-sized platelet-like single crystals of NbSe₂ via a chemical-vapor-transport technique using iodine as a transport agent. Their strain-behavior was investigated via thermal expansion and elastoresistance. Elastoresistance is determined at cryogenic temperatures by gluing samples to a piezoelectric stack (used to apply in-situ tunable strain) and measuring the induced resistance change of the sample. The different components of the elastoresistance tensor hold information, e.g., on the symmetry of ordered states and on the strain dependence of electronic fluctuations. The anisotropic thermal expansion of the crystals is measured by a high-resolution capacitance dilatometer. Generally, the thermal expansivity is given by the pressure dependence of the entropy of a material. In particular, the uniaxial pressure derivatives of a phase transition temperature can be deduced from the linear thermal expansion via thermodynamic relations, providing unique information on the anisotropic strain dependence of different ordered phases. The comparison of the elastoresistance and thermal expansion results of our 2H-NbSe₂ single crystals will be discussed.

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Understanding nanotwinned microstructures in Ni-Mn-based Heusler alloys from first-principles

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Depending on composition and chemical order, Ni-Mn-based Heusler alloys exhibit interesting functional properties, which render them useful for magnetic shape memory applications or as magnetocaloric materials. This is linked to the presence of hierarchically twinned modulated structures in martensite, which can be interpreted as adaptive, self-organized arrangement of [110]-aligned nanotwins consisting of non-modulated tetragonal building blocks as was shown previously for the paradigmatic case of stoichiometric Ni₂MnGa [1]. A band-Jahn-Teller-type reconstruction of the Fermi surface which in particular softens the [110] transversal acoustic phonons leads to a downhill transformation path from cubic austenite to nanotwinned martensite [2]. The twin interfaces are subject to competing repulsive and attractive interactions related to the frustrated antiferromagnetic coupling between neighboring Mn atoms [3].

Based on recent first-principles calculations in the framework of density functional theory, the present contribution explores the signatures of the interdependence of magnetism, chemical order and nanotwinning in Ni-Mn-based Heusler systems beyond Ni-Mn-Ga and their relevance for the functional properties. Particular emphasis will be made on off-stoichiometric compositions suitable for magnetocaloric purposes.

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Purely anharmonic charge-density wave in the 2D Dirac semimetal SnP

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Two-dimensional (2D) materials displaying charge density waves (CDWs) have been one of the main focus of research in condensed matter physics for the last decades, as their rich properties can be used for quantum-based technologies. While first investigations were devoted to bulk materials, 2D materials result more optimal for potential applications. In particular, a CDW may induce a metal-insulator transition when it couples two Dirac fermions and as a result a topological phase could arise. In this work we study such behavior in a new 2-dimensional van der Waals material, SnP, exhibiting three different CDWs. We first confirmed the stability of its bulk counterpart Sn₄P₃, both using density functional theory (DFT) calculations and by synthesizing it experimentally. The experiments also confirmed the layered structure of the compound, suggesting the structure may be synthesized down to the monolayer by exfoliation or chemical means. Despite the stability of the bulk counterpart, the monolayer presents unstable phonons at Γ , K and M, which lead to three possible charge-density-wave phases. Here, we study the occurrence of these three CDWs by analyzing the phonons with a non-perturbative treatment of anharmonicity. While all three CDWs lead to metastable insulator phases, interestingly, the ground-state structure would be unnoticed without anharmonic effects, which are very strong in the system. Ultimately, we performed a symmetry indicators based topological analysis, showing how, under strain, the phase driven by the active phonon in the K point is topologically non-trivial.

Soft phonons in CDW phase transitions from first principles

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Structural phase transitions and anomalous lattice dynamics properties are often interrelated. Very prominent examples are charge-density wave (CDW) transitions, which are typically accompanied by the presence of soft phonons. These phonons exhibit strong temperature dependencies, and become unstable at the phase transition. Density functional perturbation theory (DFPT) is a powerful tool to investigate the properties of these anomalous phonons from first principles. The momentum and displacement pattern of the soft mode is directly linked to the periodicity (commensurate /incommensurate) and symmetry reduction of the CDW phase. Because the detailed momentum structure of the electron-phonon coupling can be calculated within DFPT, it provides insight into the mechanism driving the phase transition. Furthermore, pressure/strain effects on the soft mode and thus on the phase transition can easily be analyzed. The power of this method is exemplified for various classes of CDW compounds in comparison with experimental observations [1,2].

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Field-Direction-Dependency of the Electrocaloric Effect

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The electrocaloric effect (ECE) is the adiabatic temperature change that occurs in polar materials in a varying electric field. Maximal responses are observed near the diffusionless structural phase transitions of ferroelectrics. Unlike its magnetic counterpart, the magnetocaloric effect, it is strongly tunable by the field directions. [1,2,3] However, research so far focused mainly on the high symmetric field directions, i.e. $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$, and the general behavior of the ECE in low symmetric field direction is unclear.

In this work, we study the field-direction-dependency of the ECE of the prototypical ferroelectric material BaTiO_3 , using a coarse-grained molecular dynamics simulator[4] based on a first-principles-derived effective Hamiltonian parameterized by DFT calculations. We sample the ECE in all potential field directions over a wide temperature range using the direct method. We find that the maximal responses are in the high symmetric $\langle 100 \rangle$ direction. Close to this direction, the phase stability and the ECE are particularly field-direction sensitive. We believe this finding can provide general insights into the anisotropic nature of the ECE not only for single- but also for poly-crystalline ferroelectric perovskites.

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Investigating Electronic Structures of Kagome Metals

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The Kagome metals have garnered considerable attention lately due to their unusual electronic structures. These materials have a special geometry that results in a range of instabilities, such as superconductivity, spin liquid states, and charge density waves. A particularly interesting family of non-magnetic Kagome metals is AV_3Sb_5 ($A = K, Rb, Cs$), which showcases unconventional superconductivity, charge density waves, and an intricate band topology due to nearby saddle points near the Fermi level. To better understand these materials, we conducted a computational study of their band structures and Fermi surfaces. The Lindhard susceptibility calculations were applied to evaluate the Fermi surface nesting in these compounds. We also explored the relationship between the CDW and SC states through hole doping in these systems, both experimentally and computationally. Our results show that small variations in carrier doping can significantly affect the SC and CDW order in $AV_3Sb_{5-x}Sn_x$.

Single crystal growth of Ni_2MnGa , $\text{Ni}_{48}\text{Co}_5\text{Mn}_{25}\text{Ga}_{22}$ and BaBiO_3

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For the investigation of CDW materials and CDW-related phase transitions, the preparation of high quality samples is essential. In particular, characterization methods such as neutron scattering rely on single crystalline bulk samples for studies of structure and phonon dispersion, but also transport measurements benefit from orientation-resolved measurements. In this paper, the approach of single crystal growth by the Bridgman method as well as results are presented. The focus is on half-Heusler phases and half-Heusler-based phases Ni_2MnGa and $\text{Ni}_{48}\text{Co}_5\text{Mn}_{25}\text{Ga}_{22}$, which combine magnetic as well as electronic and CDW phenomena, and on the perovskite phase BaBiO_3 . Characterizations using DSC, XRD, Laue photography and electrical transport measurements are also presented to evaluate the quality of the fabricated samples.

Spin-dependent electron entropy at phase transitions

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Recent studies have determined the electron entropy of free electrons across displacive phase transitions by detecting temperature-dependent transport properties. Exemplary materials are NiTi [1] and Ni-doped FeRh [2]. Using the Seebeck coefficient from thermopower measurements and the Hall constant from Hall experiments, the electron entropy can be derived. So far, these studies do not analyze any dependence on the spin state of the materials.

In order to discuss spin-dependent driving forces of these phase transitions, the electron entropy has to be obtained with spin sensitivity in magnetic materials. Therefore, spin-dependent Seebeck measurements have to be conducted. The anisotropy of the Seebeck coefficient with respect to the magnetic field direction will provide the information needed to derive the spin-dependent electron entropy as discussed on this poster.

Here, a detailed derivation of the spin-dependent electron entropy from anisotropic Seebeck measurements and Hall experiments is presented. Basic experimental setups for these transport experiments already exist, but have been used so far only for anisotropic Seebeck measurements at room temperature [3-5] or for tunnel-magneto Seebeck studies [6-8]. Therefore, an outlook is given for an upgrade of these experiments to study the spin-dependent entropy at phase transitions in magnetic materials, such as the Heusler compound Ni₂MnGa.

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Lattice contribution to entropy change at first order phase transition in Laves phase DyCo₂

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Laves phases are promising candidates for the gas liquefaction process at cryogenic temperatures, as they show an in temperature adjustable first-order phase transition and sizeable magnetocaloric effect [1]. Within this work, we will present nuclear forward scattering techniques to study the Dy-sublattice along the temperature driven first-order phase transition of the DyCo₂ Laves phase. We are able to resolve magnetic and electronic properties by nuclear forward scattering (NFS) [2]. At the first-order phase transition, the isothermal entropy change has contributions of magnetic, electronic and lattice degrees of freedom [3]. To resolve the lattice contribution to the total entropy change, we performed nuclear resonant inelastic X-ray scattering (NRIXS) experiments, from which we extract the ¹⁶¹Dy-partial vibrational density of states [4]. Via thermodynamic relations it is then possible to calculate the corresponding vibrational entropy at the respective temperatures [5]. From NFS data we find changes in electronic and magnetic properties within the magnetic low temperature phase, which can be correlated to changes in the ¹⁶¹Dy-partial VDOS, but are not responsible for changes in the vibrational entropy. Changes at other contributions of the ¹⁶¹Dy-partial VDOS occur at higher temperatures which can be correlated with the change in vibrational entropy at the first-order phase transition. We acknowledge financial support from DFG through CRC/TRR 270 HoMMage. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

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Chiral domains in Tantalum disulfide

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It was recently observed that the nearly commensurate charge density phase in TaS₂ hosts chiral domains of commensurate charge order [1]. Here we present a Ginsbourg-Landau theory explaining the emergence of this chirality from a competition between the coupling of the charge order with the lattice and the electronic susceptibility.

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Terahertz signatures of the martensitic phase transformation in NiTi alloys

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Nickel-Titanium alloys are well known shape memory alloys that feature a martensitic phase transition. So far, the phase transformation in this system has been attributed to softening of the phonon. However, the role of the electrons within this process was not considered important. Here we present temperature-dependent reflectivity spectra in the terahertz (THz) range for Ni₅₁Ti₄₉ and Ni_{51.2}Ti_{48.8} [1]. The spectral range exploited in this study is far below the lowest frequency of the optical phonon mode in NiTi (~7.5 THz), thus one can trace the pure temperature-dependent electronic response. As the temperature is reduced below the phase change temperature, the reflectivity decreases rapidly by about 2%, which is attributed to a reduction of the free-carrier concentration caused by the formation of a charge-density wave. When the temperature is reduced further, the reflectivity partially recovers as the decrease in carrier density is compensated by the increased mobility at lower temperature. The observed THz signatures are in agreement with dc transport characterization, i.e. resistivity and Hall measurement.

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Transport-magnetism correlation in layered perovskite manganite (LaCaBiMn₂O₇)

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This study provides a look at the magnetoresistance (MR) and transport characteristics of the LaCaBiMn₂O₇ material. At a magnetic field of 5 T, our compound has a significant MR impact of 55% around T_{MI}. and the highest TCR value of 0.89 K⁻¹. The unusual behavior of the resistivity in the 2 K < T < 25 K temperature range can be explained by a combination of the effects of weak localization, electron-electron scattering, and electron-phonon scattering. As the magnetic field is increased, these combined effects become less visible. We have used the percolation theory, which is based on ferromagnetic-metallic and paramagnetic-insulator phase segregation. To examine the electrical resistivity at all temperatures, with a focus on the region around the T_{MI} peak temperature. The correlation between those two properties, -ΔS_M as a magnetic parameter and ρ as an electrical parameter has also been investigated. The magnetic entropy change -ΔS_M was estimated using the resistivity curves observed over the complete temperature range of 2 K-400 K for a variety of applied magnetic fields ρ (H, T), and the findings were equivalent to those predicted using the resistivity curves M (H, T), around T_C.

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First-order antiferromagnetic transitions in CaMn_2P_2 and SrMn_2P_2 single crystals containing corrugated-honeycomb Mn sublattices

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CaMn_2P_2 and SrMn_2P_2 are insulators that crystallize in the trigonal CaAl_2Si_2 -type structure. Magnetic susceptibility $\chi(T)$ and heat capacity measurements reveal a strong first-order antiferromagnetic (AFM) transition in CaMn_2P_2 at $T_N = 69.8(3)$ K and a weak first-order AFM transition in SrMn_2P_2 at $T_N = 53(1)$ K [1]. The $\chi(T)$ data for both compounds exhibit nearly isotropic and temperature-independent behavior below T_N . NMR measurements indicate a commensurate AFM structure for CaMn_2P_2 and an incommensurate one for SrMn_2P_2 . CaMn_2P_2 and SrMn_2P_2 are rare examples where an AFM transition in zero-magnetic field is thermodynamically of first order. A possible mechanism that drives a magnetic transition to be of first order in CaMn_2P_2 is its coupling to a structural transition. These first-order AFM transitions are unique among the trigonal $(\text{Ca}, \text{Sr}, \text{Ba})\text{Mn}_2(\text{P}, \text{As}, \text{Sb}, \text{Bi})_2$ compounds, which mostly exhibit second-order AFM transitions [2]. Determining the mechanism for the first-order transitions may lead to development of new materials of technological interest.

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Investigation of solid-state interface interactions in FeSe/TiSe₂ multilayers as example for dichalcogenide systems

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Chalcogenides became a prominent class of materials in various fields of solid-state physics. Prominent examples are Bi_xSb_{1-x}Te₃ compounds in thermoelectrics or topological materials. Bi₂Te₃ was the first material, where topological surface states were shown. TiSe₂ as part of this class of materials has been reported to show a charge density wave transition. FeSe is known to show superconductivity at low temperatures (<10K) connected with the occurrence of a nematic phase below 100 K. However, the interplay between charge density wave phase and the superconductivity is not fully understood. We work on the synthesis of these two compounds via magnetron sputtering in multilayer systems and want to investigate the interplay between the charge density wave phase and the superconducting phase. We show a report on the state of the work in progress on the sputtering process and first characterization of the films.

Addressing the spin-valley flavors in moiré mini-bands of MoS₂

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In the last decade, the evolution of van der Waals material systems has provided a multitude of options to manipulate, control, and engineer materials properties to various needs by combination, proximity, and twisting. Moiré superlattices formed as a result of lattice mismatch or twist angle modify the electronic structure to create flat bands and host exotic correlated electron phases [1]. Transition metal dichalcogenides relax the stringent magic angle condition for flat band formation, unlike graphene [2,3]. Our transport spectroscopy measurements and analysis reveal a correlation-driven phase transition and the emergence of discrete mini-bands in MoS₂ moiré superlattices that remained elusive so far. We resolve these mini-bands arising from quantum mechanical tunnelling through Schottky barriers between the MoS₂ and its metallic leads. Energy scales deduced from a first approach exhibit an astounding agreement with our experimental observations. The behaviour under thermal activation suggests a Lifshitz phase transition at low temperatures that is driven by a complete spin-valley symmetry breaking. These intriguing observations bring out the potential of twisted MoS₂ to explore correlated electron states and associated physics.

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NiTi growth by the micro pulling down method

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Many characterization methods require single crystalline samples of high crystalline quality. Crystals of such quality are hardly accessible, especially for intermetallic phases. For the preparation of such single-crystalline samples, several methods can be considered, such as the Czochralski-method or the Bridgman-method. However, most established single crystal growth methods are relatively long term processes and thus the variation of parameters is time consuming. We offer the solution to this problem by a relatively unknown method for crystal growth, the micro pulling down (μ pd) method. A μ pd-setup was designed and is set up at Bielefeld University. This method shows high flexibility and short production times. As the crystal is grown in the μ pd-method from the bottom of the melt, oxide contamination is reduced. Special emphasis during the design of the μ pd-setup was payed to the atmospheric control, since intermetallic phases are extremely susceptible to oxidation. As a representative of the intermetallic phases, NiTi was grown. Additionally, NiTi is a potential model system for charge density wave phases. First characterizations on the obtained samples were performed and are discussed in context of the literature.

Broadband dielectric spectroscopy of BaTiO₃-based relaxor ferroelectrics

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The relaxor behavior of BaTiO₃ (BTO)-based solid solutions has been extensively studied due to their potential applications in energy harvesting, electrocalorics and multi-layered capacitors. The main focus is on the homovalent substituted barium titanate. The most common substitution for the B-site titanium ion are carried out with zirconium, cerium and tin which have larger ionic radius than titanium itself. These ions are ferroelectrically-inactive. The increase of concentration of substitutional species suppresses the ferroelectric phase by merging three phase transitions of barium titanate and developing of a broad relaxor-like dielectric dispersion.

It has been argued that BTO-based relaxors have features that are more common to the dipolar/spin glasses [1,2]. The broadband dielectric spectroscopy of BaTi_{1-x}Zr_xO₃ revealed that the mean relaxation time obeys Arrhenius law (i. e. the freezing temperature is 0 K) [3].

In this contribution we present the dielectric results of BaTi_{1-x}Sn_xO₃ ($x = 0.15; 0.2; 0.25; 0.3$) in 1 mHz – 1 THz frequency range. The system will be compared to the canonical Pb-based relaxors and other homovalent-substituted BTO relaxors. The presence of Vogel-Fulcher freezing phenomena will be discussed.

Additionally, the dielectric properties of BTO doped with tin (Sn⁴⁺) and cerium (Ce⁴⁺) that exhibit relaxor-like behaviour will be discussed. The broad frequency range from 1 mHz to 1 THz has been covered to determine the relaxation time in these materials to identify Vogel-Fulcher freezing. Additionally, the polarization and strain hysteresis will be discussed to understand if ferroelectric phase can be induced.

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Elastoresistance of the antiferromagnetic (Ca,Sr)Co₂As₂ system in different symmetry channels

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Elastoresistance is a powerful and increasingly common method for manipulating and studying the properties of correlated electron systems. It has been particularly interesting to study the nematic state of several unconventional superconductors with elastoresistance [1,2]. In the current study, we present the method of elastoresistance and how it can be applied to study various phase transitions. It is applied to the itinerant antiferromagnet (Ca,Sr)Co₂As₂ that shows a collapsed to uncollapsed-tetragonal structural transition upon Sr substitution [3]. We show how uniaxial or biaxial strain in different symmetry channels affects electrical resistance. The results are discussed in the context of competing magnetic fluctuations in SrCo₂As₂.

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Ab initio DFT investigation of the inversion-breaking Weyl semimetal PtBi2

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PtBi2 is a newly discovered type-I Weyl semi-metal, displaying extremely high magnetoresistance[1] and unusual superconducting properties [2,3]. Given the rich physics of this compound, we performed DFT investigations of its electronic band structure, to understand and characterize its topological aspects. Here, we report and discuss calculations for bulk, finite and semi-infinite system, showing how the surface Fermi arcs carry significant weight very close to the Fermi level.

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