

2ND WORKSHOP FLOATING ZONE TECHNIQUE DRESDEN

4-6 APRIL 2016

Venue:

Leibniz Institute for Solid State and Materials
Research Dresden, Germany

Invited speakers in alphabetical order:

- A. Erb (Walther-Meißner-Institut, DE)
- A. Isaeva (TU Dresden, DE)
- S. Khim (MPI CPfS Dresden, DE)
- F. Lichtenberg (ETH Zürich, CH)
- J. F. Mitchell (Argonne NL, US)
- R. C. Morrow (IFW Dresden, DE)
- E. Pomjakushina (Paul Scherrer Institute, CH)
- D. Prabhakran (Oxford University, GB)
- A. Prokofiev (TU Wien, AT)
- S. Wilson (UC Santa Barbara, US)
- B. Yan (MPI CPfS Dresden, DE)

Additional information and registration:
www.crystalgrowth.info

THIS WORKSHOP IS DEDICATED TO DR. GÜNTER BEHR (D. 2010)



Leibniz Institute
for Solid State and
Materials Research
Dresden



SCIDRE
SCIENTIFIC INSTRUMENTS DRESDEN GMBH

Venue

Our 2nd Workshop "Floating Zone Technique" will take place at IFW Dresden e. V., which is located in the center of the main campus of Technische Universität (TU) Dresden. The IFW Dresden is in the south of Dresden 2,5km from the city center.

Access

By car

Take the motorway A4, at interchange Dresden – West change to the A17 to Praha. Exit at Dresden – Südvorstadt. Follow the road into town for around 2 km up to the campus of the TU Dresden. Turn left into the Mommsenstraße at the end of which is the Helmholtzstraße.

From the airport or by train or tram

From the airport Dresden – Klotzsche take the city-railway (S-Bahn S2) to the Dresden Main Station (Dresden – Hauptbahnhof).

From the Dresden Main Station take the tram **No. 3 (destination Coschütz)** or **No. 8 (destination Südvorstadt)**, two stops to "**Nürnberger Platz**". (fare: Preisstufe 1)

Then by feet turn from Münchner Straße into Helmholtzstraße and follow almost up to Nöthnitzer Straße.

Locations of main events

Workshop and Poster Session:

IFW Dresden, Room D2E.27 (house D, 2nd floor, room 27), Helmholtzstraße 20, 01069 Dresden

Lunch:

You can choose to have lunch at our institute restaurant located in ground level House D or you can go to Alte Mensa, Mommsenstraße 13 which is across the street opposite from IFW Dresden.

Dinner on own expenses on April 4th, 2016:

Café Bliebig, Liebigstraße 24, 01187 Dresden, from the IFW Dresden you walk down Helmholtzstraße until you cross Liebigstraße and turn right. The restaurant is located on the left side of the street (approx.. 10 min)

Conference Dinner on April 5th, 2016:

Homage, Wasaplatz 1, 01219 Dresden

From IFW Dresden you can go up to Nöthnitzer Straße to the bus stop. Take **no. 85 (destination Striesen)** and hop off "**Wasaplatz**" (appr. 11 min.)

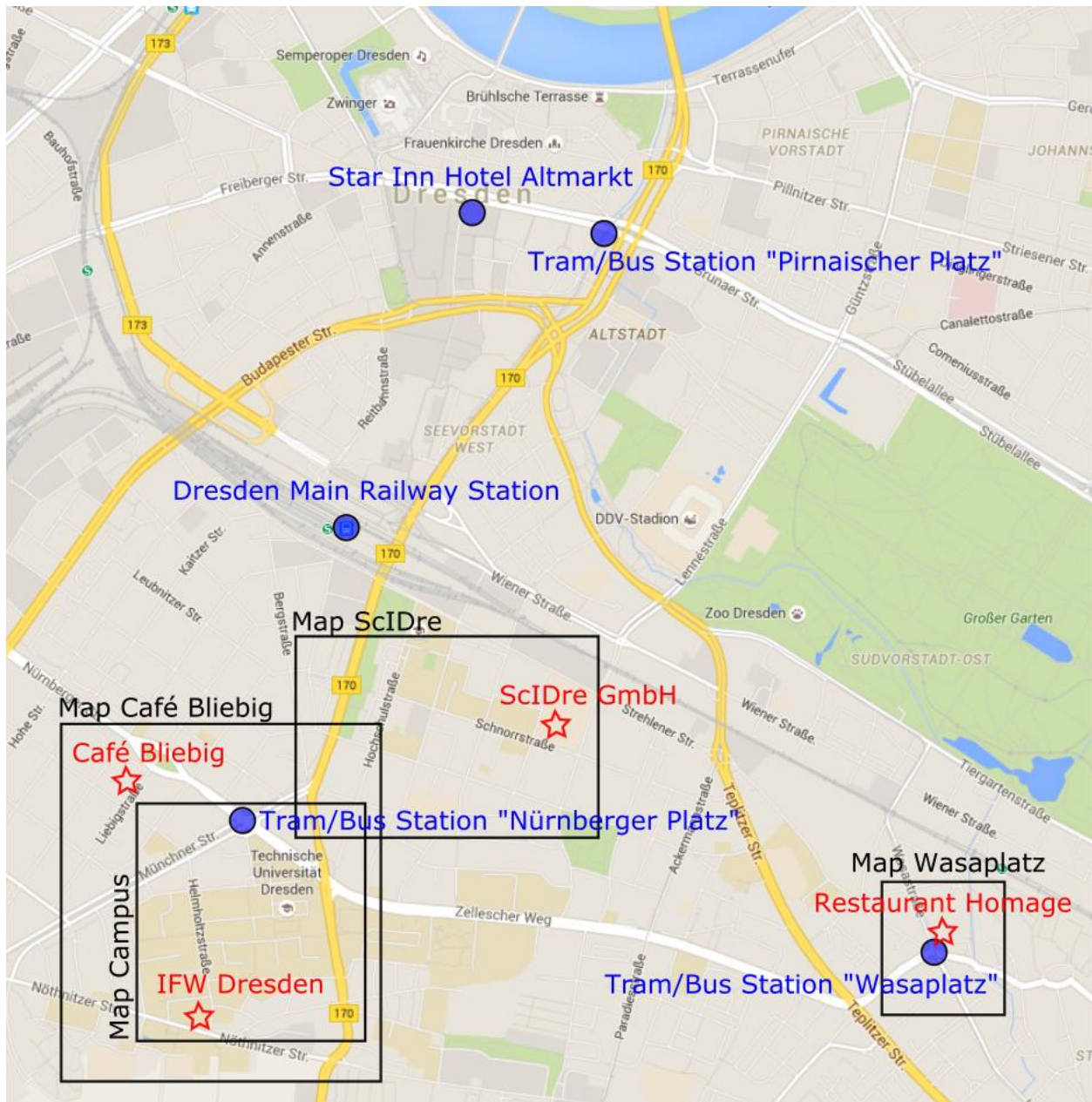
From Hotel at Altmarkt:

Walk to Pirnaischer Platz and take **bus no. 75 (destination Goppeln)** and hop off "**Wasaplatz**" (appr. 10 min)

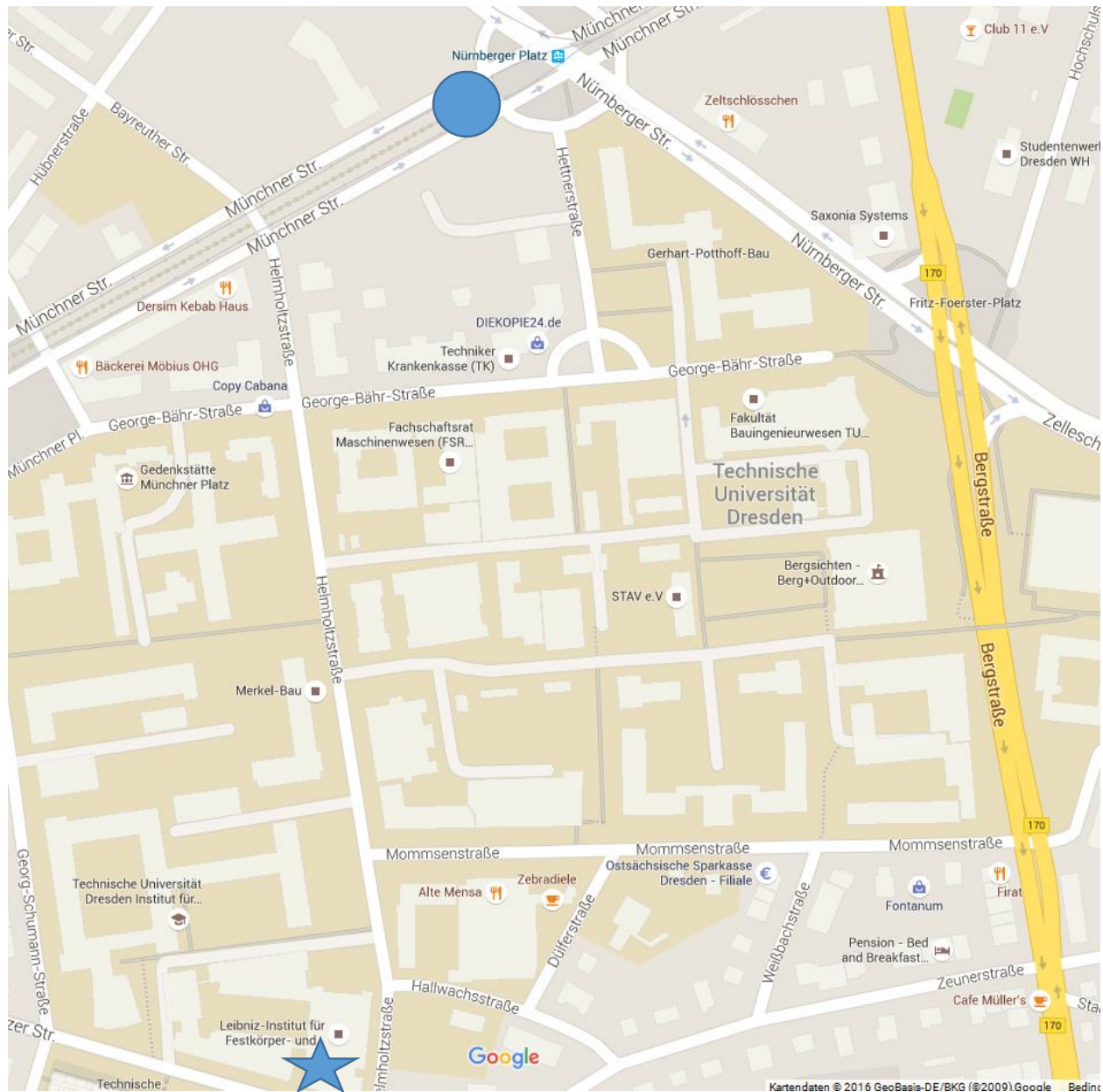
WLAN connection:

Please connect yourself to following network: "FloatingZone"

Overview Map Dresden City



Map Campus

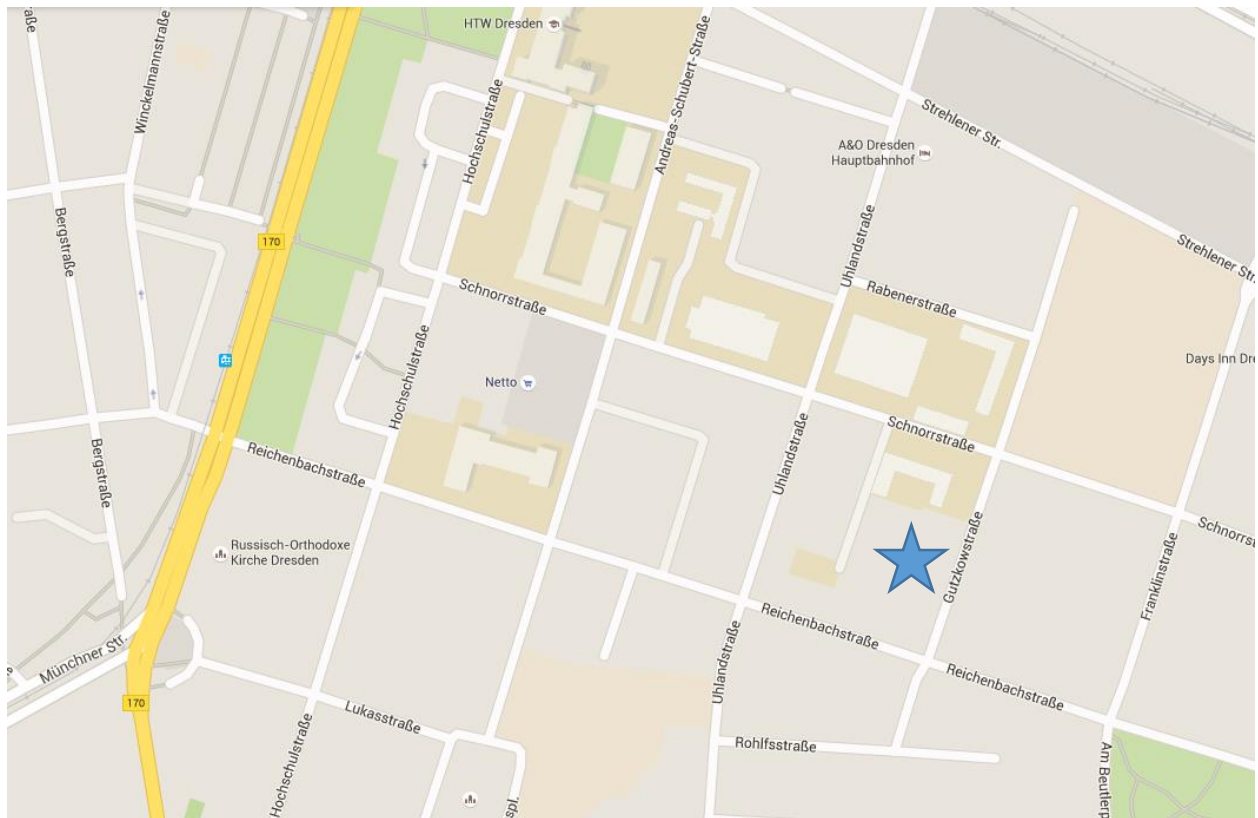


IFW Dresden



Tram #3 Stop "Nürnberger Platz"

Map ScIDre GmbH (Scientific Instruments Dresden)

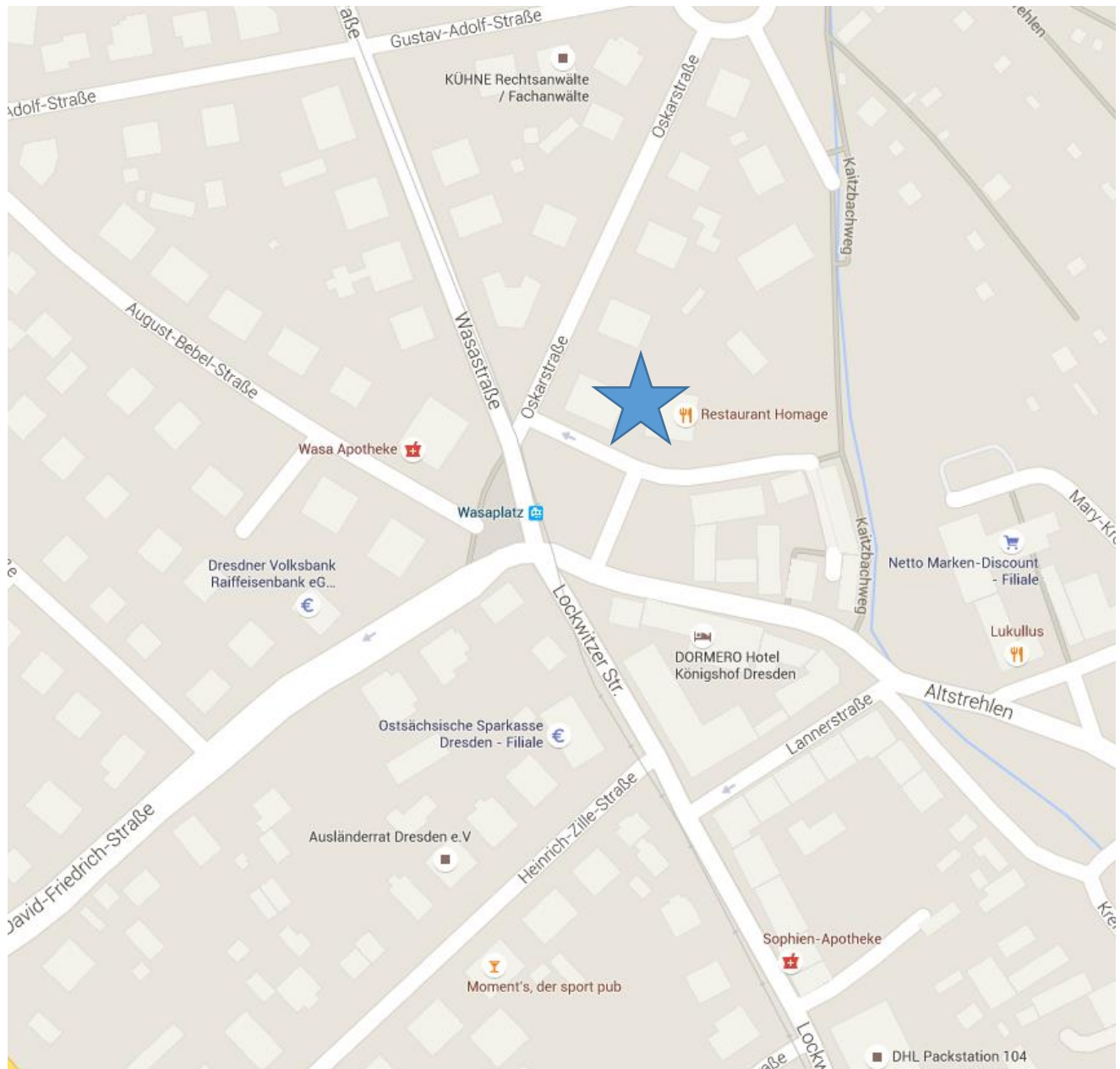


Location Scientific Instruments Dresden GmbH

Gutzkowstraße 30, 01069 Dresden

We will provide a transport from the IFW to the ScIDre location.

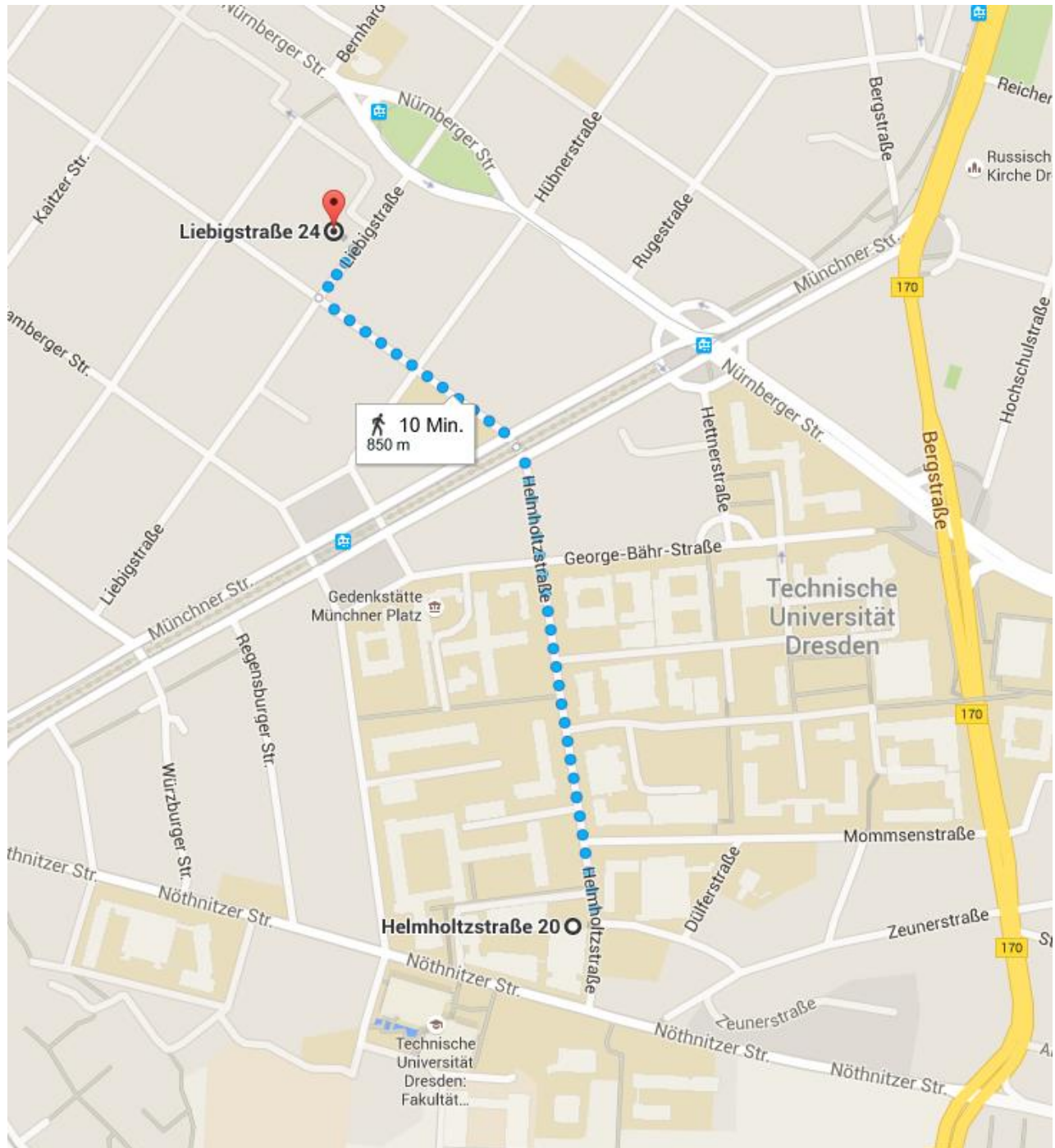
Map Wasaplatz



Restaurant Homage

Getting back to the city centre you can catch bus no. 75 (direction Pirnaischer Platz), tram no. 9 (direction Kaditz) or bus no. 61 (direction Löbtau) to get back to Nürnberger Platz.

Map Café Bliebig



Public transport

For getting around in Dresden you can check the brochures "Linienetz" and "Comfortable: bus and rail travel in Dresden" which you can find in your workshop bags.

Committee

Local Organizers

- Dr. Sabine Wurmehl, IFW Dresden
- Dipl.-Ing. (FH) Robert Schöndube, SciDre GmbH
- Dr. Paul Sass, SciDre GmbH

Secretary

- Katja Schmiedel, IFW Dresden

program

Monday, April 4th, 2016

time	speaker and title of contribution/event	session chair
12:00-01:00	registration and get together with coffee and snacks	
01:00-01:15	welcome	
01:15-02:00	Ekaterina Pomjakushina (invited talk) "Complex metal oxides and related materials grown by TSFZ: an overview of 12 years crystal growth activity at Paul Scherrer Institute"	oral session I: complex transition metal oxides (chair: J. Mitchell)
02:00-02:20	Alma Dorantes "Magnetoresistance of the electron-underdoped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$"	
02:20-03:05	Andreas Erb (invited talk) "Single crystal growth of various oxide materials for basic research and applications"	
03:05-05:00	poster session with coffee	
06:30-open end	dinner Café Bliebig (at own expenses)	

Tuesday, April 5th, 2016

time	speaker and title of contribution/event	session chair
09:00-09:45	Dharmalingam Prabhakaran (invited talk) "Floating Zone Growth – Challenges"	oral session II: role of stoichiometry and ordering (chair: A. Erb)
09:45-10:30	Stephen Wilson (invited talk) "Exploring the physical properties of a model correlated electron cathode material"	
10:30-11:00	coffee break	
11:00-11:45	Andrej Prokofiev (invited talk) "Floating zone growth of rare earth containing clathrates"	oral session III: intermetallics (chair: W. Löser)
11:45-12:05	Ahmad Omar "Towards a novel half-metallic ferromagnet in the $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$ Heusler compounds"	
12:05-12:25	Katharina Weber "Growing single crystals of peritectic YFe_4Ge_2 "	
12:25-12:45	Georg Benka "UHV-compatible preparation chain for high-purity single crystals of transition metal and rare earth compounds"	
12:45-02:15	lunch at mensa	
02:15-03:00	Frank Lichtenberg (invited talk) "Melt-grown synthesis and structural and physical properties of $A_nB_n\text{O}_{3n+2} = \text{ABO}_x$ type materials and other perovskite-related layered oxides"	oral session IV: Ruddlesden Popper phases and other perovskite related materials (chair: K. Conder)
03:00-03:45	John Mitchell (invited talk) "Charge Stripes in Quasi-Two-Dimensional Trilayer Nickelate $\text{La}_4\text{Ni}_3\text{O}_8$ "	
03:45-04:00	Paul Sass "Ideas and future requirements for FZ technique"	
04:00-04:30	coffee break	
04:30-05:30	Tentative: Lab tour IFW and /or scidre	
06:30- open end	conference dinner	

Wednesday, April 6th, 2016

time	speaker and title of contribution/event	session chair
09:00-09:45	Ryan C. Morrow (invited talk) "Superexchange Interactions in Double Perovskite Osmates"	oral session V: novel materials I (chair: S. Wurmehl)
09:45-10:30	Anna Isaeva (invited talk) "Crystal growth of new topological insulators in bismuth-halide and related systems"	
10:30-11:00	coffee break	
11:00-11:45	Binghai Yan (invited talk) "Topological surface states and chiral magneto-transport in TaAs-type of Weyl"	oral session VI: novel materials II (chair: A. Isaeva)
11:45-12:30	Seunghyun Khim (invited talk) "A new Type-II Weyl semi-metal candidate TaIrTe₄"	
12:30-12:45	discussion	Chair: S. Wurmehl
12:45-12:50	farewell	
Up from 12:50	lunch at mensa	

abstracts

**oral session I: complex transition metal oxides
(chair: J. Mitchell)**

01:15-02:00	Ekaterina Pomjakushina (invited talk) "Complex metal oxides and related materials grown by TSFZ: an overview of 12 years crystal growth activity at Paul Scherrer Institute"
02:00-02:20	Alma Dorantes "Magnetoresistance of the electron-underdoped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$"
02:20-03:05	Andreas Erb (invited talk) "Single crystal growth of various oxide materials for basic research and applications"

Complex metal oxides and related materials grown by TSFZ: an overview of 12 years crystal growth activity at Paul Scherrer Institute

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Artificially grown single crystals are very important materials for many applications and also for research purposes. The Traveling Solvent Floating Zone (TSFZ) Method is a complementary method to other well-known crystal growth techniques such as Verneuil, Bridgman, Czochralski and direct crystallization from melt/flux. It is a great tool for researchers looking for novel materials with unique magnetic, electrical and optical properties.

Our group of Solid State Chemistry at Paul Scherrer Institute is equipped with optical furnace (Model: FZ-T-10000-HVI-VP-PC, Crystal Systems Corp. Japan) already since twelve years. In my talk I will present some challenging examples of crystal growth done during these years: layered cobaltites with a general formula $\text{ReBaCo}_2\text{O}_{5+x}$ [1], strontium copper borate ($\text{SrCu}_2(\text{BO}_3)_2$), spin-ladder compounds $\text{Bi}(\text{Cu}_{1-x}\text{Zn}_x)_2\text{PO}_6$ [2] and $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ with $x > 12$ [3]. Large single crystals of $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ with $x > 12$ were successfully grown using in-house modified high pressure traveling floating zone method.

[1] M. Stingaciu, E. Pomjakushina, H. Grimmer, M. Trottman, K. Conder. Crystal growth of $\text{Tb}_{0.9}\text{Dy}_{0.1}\text{BaCo}_2\text{O}_{5+\delta}$ using travelling solvent floating zone method. J. Cryst. Growth **310** (2008) 1239

[2] S. Wang, E. Pomjakushina, T. Shiroka, G. Deng, N. Nikseresht, Ch. Rüegg, H.M. Rønnow, K. Conder. Crystal growth and characterization of the dilutable frustrated spin-ladder compound $\text{Bi}(\text{Cu}_{1-x}\text{Zn}_x)_2\text{PO}_6$. J. Cryst. Growth **313** (2010) 51

[3] G. Deng, D. Mohan Radheep, R. Thiyagarajan, E. Pomjakushina, S. Wang, N. Nikseresht, S. Arumugam, K. Conder. High oxygen pressure single crystal growth of highly Ca-doped spin ladder compound $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ ($x < 12$). J. Cryst. Growth **327** (2011) 182

Magnetoresistance of the electron-underdoped cuprate superconductor $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$

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$\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) is an electron-doped high temperature superconductor (HTSC) from the 214 cuprate family. The latter have the general formula $Ln_{2-x}A_x\text{CuO}_4$ (Ln = rare earth metal, A = Ca, Sr, Ce, etc.). The parent compound is a Mott insulator and through the insertion of charge carriers, superconductivity can be achieved. In order to become superconducting, the electron-doped cuprates require a post-growth annealing treatment which removes the apical oxygen in the T' structure [1]. According to literature, superconductivity is restricted to a doping range from $x = 0.13$ to $x = 0.18$ with a transition temperature $T_{c,opt} = 25$ K at optimal doping $x_{opt} = 14.5$ [2].

In the parent compound, the Cu^{2+} spins order in an antiferromagnetic structure (AF) and in contrast with the hole-doped cuprate superconductors, there is no definite separation between the AF and superconducting (SC) regions of the phase diagram. It is not clear if these two states coexist or if there is an intrinsic phase separation. The magnetic structure shows two basic configurations, the collinear and noncollinear structures. In the collinear structure the spins point either parallel or antiparallel to a single direction, and in the noncollinear the spins in adjacent layers are orthogonal [3]. By the application of a magnetic field a spin-flop transition from noncollinear to collinear structure can be induced.

The Traveling Solvent Floating Zone method (TSFZ) was used to grow NCCO underdoped single crystals, $x = 0.09$ - 0.13 . Evidence of superconductivity, at least in a part of the crystal volume, was found for every dopant concentration including $x = 0.09$. We found that T_c and the SC volume fraction present a wide variation near $x = 12.5$; however, superconductivity at $x = 0.12$ is more reproducible.

In order to investigate the possible coexistence of the AF and SC orders we have measured the angular dependent magnetoresistance (MR) on NCCO single crystals with $x = 0.10$, 0.12 and 0.125 . The jump in the MR with B around the Cu–O–Cu direction coincides with the spin-flop transition, thus we can observe the coexistence of long range AF and SC states in our samples.

[1] N. Armitage, P. Fournier und R. L. Greene, „Progress and perspectives on electron-doped cuprates,“ *Reviews on Modern Physics*, **82** (2010) 2421

[2] M. Lambacher, T. Helm, M. Kartsovnik and A. Erb, "Advances in single crystal growth and annealing treatment of electron-doped HTSC," *Europ. Phys. J. Special Topics* **188** (2010) 61

[3] T. Wu, C. H. Wang, G. Wu, D. F. Fang, J. L. Luo, G. T. Liu und X. H. Chen, „Giant anisotropy of the magnetoresistance and the 'spin valve' effect in antiferromagnetic $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$,“ *J. Phys. Condensed Matter* **20** (2008) 275226

**Single crystal growth of various oxide materials
for basic research and applications**

Andreas Erb

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The development of both the FZ and the TSFZ technique for the use of oxide single crystals offers the possibility to grow not only stoichiometric but also solid solution compounds in very high quality. While not possible for all materials, the application of this growth method is not only highly effective but also a very cost efficient method since no expensive and sometime polluting crucibles are needed and basically all material is crystallized even in the case of non-congruently melting compounds.

We will present several examples for the use of this technique for the growth of crystals for basic research and applications.

Poster session

Structural and magnetic properties of $\text{Sr}_2\text{Y}_{1+x}\text{Ir}_{1-x}\text{O}_6$

Gizem Aslan Cansever^{1*}, Maximilian Geyer¹, Christian G.F. Blum¹, Sebastian Gass¹, Kaustuv Manna³, Franziska Hammerath^{1,2}, Laura T. Corredor¹, Andrey Maljuk¹, A.U.B. Wolter¹, Sabine Wurmehl^{1,2}, and Bernd Büchner^{1,2}

¹IFW Dresden, Institute for Solid State Research, 01171 Dresden, Germany

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Ir-based materials have attracted a lot of attention because of the competition between the spin-orbit coupling, Coulomb interaction and crystal field [1]. Sr_2YIrO_6 double perovskites with Ir^{+5} ($5d^4$) ions are generally considered to have a nonmagnetic ground state ($J=0$). However, Sr_2YIrO_6 double perovskites have been reported to exhibit long-range magnetic order at low temperature and the distorted IrO_6 octahedra were discussed to cause the magnetism in this compound [2]. In this study $\text{Sr}_2\text{Y}_{1+x}\text{Ir}_{1-x}\text{O}_6$ materials were investigated in relation to structural and magnetic properties with varying Y and Ir concentrations. The samples were prepared by solid-state chemical reaction method. Magnetic susceptibility measurements were performed down to 0.4 K.

[1] G. Khaliullin, Phys.Rev. Lett. 111, 197201 (2013).

[2] G. Cao et al. Phys. Rev. Lett. 112,056402 (2014).

Crystal growth and physical properties of Na-doped BaFe₂As₂ superconducting single crystals

S. Aswartham^{1*}, M. Abdel-Hafiez¹, D. Bombor¹, A. U. B. Wolter¹, M. Kumar¹, C. Hess¹,
D. V. Evtushinsky¹, V. B. Zabolotnyy¹, A. A. Kordyuk¹, T. K. Kim^{1,2}, S. V. Borisenko¹, F.
Waßer,³ A. Schneidewind,³ Y. Sidis,³ M. Braden³, S. Wurmehl¹ and B. Büchner¹

¹Leibniz Institute for Solid State and Materials Research, D-01069 Dresden, Germany

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Single crystals of Ba_{1-x}Na_xFe₂As₂ with $x = 0, 0.25, 0.35, 0.4$ were grown using a self-flux high temperature solution growth technique. The superconducting and normal state properties were studied by temperature dependent magnetic susceptibility, electrical resistivity and specific heat revealing that the magnetic and structural transition is rapidly suppressed upon Na-substitution at the Ba-site in BaFe₂As₂, giving rise to superconductivity. A superconducting transition as high as 34 K is reached for a Na-content of $x=0.4$. The positive Hall coefficient confirms that the substitution of Ba by Na results in hole-doping similarly to the substitution of Ba by K. Angle resolved photoemission spectroscopy was performed on all Ba_{1-x}Na_xFe₂As₂ crystals. The Fermi surface of hole-doped Ba_{1-x}Na_xFe₂As₂ is to high extent the same as the Fermi surface found for the K-doped sister compounds, suggesting a similar impact of the substitution of Ba by either K or Na on the electronic band dispersion at the Fermi level. Our single-crystal neutron-diffraction experiments on $x = 0.35$ single crystal shows spin reorientation along the along the c direction at 46 K.

Ba₂YIrO₆ : A cubic double perovskite material with Ir⁵⁺ ions

T. Dey¹, A. Maljuk^{1*}, D.V. Efremov¹, O. Kataeva¹, S. Gass¹, C.G.F. Blum¹, F. Steckel¹,
D. Gruner¹, T. Ritschel¹, A.U.B. Wolter¹, J. Geck¹, C. Hess^{1,2}, S. Wurmehl^{1,2},
and B. Büchner^{1,2}.

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Materials with a $5d^4$ electronic configuration are generally considered to have a nonmagnetic ground state ($J=0$). Interestingly, Sr₂YIrO₆ (Ir⁵⁺ having $5d^4$ electronic configuration) was recently reported to exhibit long-range magnetic order at low temperature and the distorted IrO₆ octahedra were discussed to cause the magnetism in this material. Hence, a comparison of structurally distorted Sr₂YIrO₆ with cubic Ba₂YIrO₆ may shed light on the source of magnetism in such Ir⁵⁺ materials with $5d^4$ configuration. Besides, Ir⁵⁺ materials having $5d^4$ are also interesting in the context of recently predicted excitonic types of magnetism. Here we report on crystal growth and single-crystal-based analysis of the structural, magnetic, and thermodynamic properties of Ba₂YIrO₆. We observe that in Ba₂YIrO₆ for temperatures down to 0.4 K, long-range magnetic order is absent but at the same time correlated magnetic moments are present. The origin of these moments is presently unclear.

Search for magnetocaloric materials in the Co-Mn-Si system

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Materials, which show a high magnetocaloric effect are interesting for modern cooling systems because of their solid state. The magnetocaloric effect occurs at a magnetic phase transition. Some materials show a metamagnetic transition (e.g. ferromagnetic to antiferromagnetic) and often a structural transition at the same time, which together induce high entropy changes. In this studies we were able to find such a meta-magnetic transition in the Co-Mn-Si system. For this we prepared a sample series between the ferromagnetic Co_2MnSi and the antiferromagnetic Mn_3Si parent compound by changing the Co-Mn relationship. Every sample of this series $\text{Co}_{2-x}\text{Mn}_{1+x}\text{Si}$ (except the parent compound Co_2MnSi) is a multiphase material. Due to this, the different magnetic nature of the phases lead to rival interactions, which induce meta-magnetism in some samples. The phase MnCoSi plays an important role for structural and magnetic properties in those samples.

**The influence of p- and n-doping on the intrinsic properties
of the Heusler compound Fe₂VAI**

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The Heusler compound Fe₂VAI is considered as a non-magnetic thermoelectric material. In this work, we studied the intrinsic properties of the Heusler compound Fe₂VAI and the influence of p- and n-doping on the intrinsic materials properties of the corresponding Si and Ti doped compounds using single crystals. Electron back scattering diffraction reveals the presence of a V-rich secondary ferromagnetic phase in particular in crystals with Si and in the parent compound, which could be further confirmed by TEM investigations. The depletion of V from the Fe₂VAI matrix apparently leads to localized Fe moments and also to ferromagnetism in the corresponding samples. This were analyzed by means of NMR and SQUID- measurements. Interestingly, the sample with Ti and less V depletion shows a significant enhancement of the figure of merit compared to the other samples.

Tuning the magnetic properties of new layered iron chalcogenides $(\text{BaF})_2\text{Fe}_{2-x}\text{Q}_3$ ($\text{Q}=\text{S}, \text{Se}$) by changing the defect concentration on the iron sublattice

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Low-dimensional compounds of transition-metal elements continue to be the focus of diverse scientific studies because of a multitude of interesting electrical and magnetic properties, such as high-temperature superconductivity [1], colossal magnetoresistance [2] and thermoelectricity [3]. Effecting and controlling ferromagnetic-like properties in semiconductors has proven to be a complex problem, especially when approaching room temperature.

Here we demonstrate the important role of defects in the magnetic properties of semiconductors by reporting the structure and properties of the iron chalcogenides $(\text{BaF})_2\text{Fe}_{2-x}\text{Q}_3$ ($\text{Q} = \text{S}, \text{Se}$), which exhibit anomalous magnetic properties that are correlated with defects in the Fe-sublattice. The compounds form in both long-range ordered and disordered polytypes of a new structure typified by the alternate stacking of fluorite $(\text{BaF})_2^{2+}$ and $(\text{Fe}_{2-x}\text{Q}_3)^{2-}$ layers. The latter layers exhibit an ordered array of strong Fe-Fe dimers in edge-sharing tetrahedral dimers. Given the strong Fe-Fe interaction, it is expected that the Fe-Fe dimer is antiferromagnetically coupled, yet crystals exhibit a weak ferromagnetic moment that orders at relatively high temperature: below

280 – 315 K and 240 - 275 K for the sulfide and selenide analogs, respectively. This transition temperature positively correlates with the concentration of defects in the Fe-sublattice as determined by single crystal x-ray crystallography. Our results indicate that internal defects in $(\text{Fe}_{2-x}\text{Q}_3)$ layers play an important role in dictating the magnetic properties of newly discovered $(\text{BaF})_2\text{Fe}_{2-x}\text{Q}_3$ ($\text{Q} = \text{S}, \text{Se}$), which can yield switchable ferromagnetically ordered moments at or above room temperature.

References:

- [1] Sheng, Z. *et al.*, *Nature* **332**, 138 (1988).
- [2] Asamitsu, A. *et al.*, *Nature* **373**, 407 (1995).
- [3] Chung, D. Y. *et al.* *Science* **287**, 1024 (2000).
- [4] Sturza M. *et al.*, *Chem. Mater.* **27**, 3280 (2015).

Cs vacancy ordering and properties of phase separated $\text{Cs}_x\text{Fe}_{2-y}\text{Se}_2$

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S. Rosenkranz¹, M. G. Kanatzidis^{1,4}

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By simultaneously displaying magnetism and superconductivity in a single phase, the iron-based superconductors provide a model system for the study of magnetism's role in superconductivity. The class of intercalated iron selenide superconductors is unique among these in having the additional property of phase separation and coexistence of two distinct phases—one majority phase with iron vacancy ordering and strong antiferromagnetism, and the other a poorly understood minority microscopic phase with a contested structure. Adding to the intrigue, the majority phase has never been found to show superconductivity on its own while the minority phase has never been successfully synthesized separate from the majority phase.

In order to better understand this minority phase, a series of high-quality $\text{Cs}_x\text{Fe}_{2-y}\text{Se}_2$ single crystals with ($0.8 \leq x \leq 1$; $0 \leq y \leq 0.3$) were grown and studied. At high temperature, a 122 - type structure with random iron vacancies undergoes a complex iron vacancy ordering scheme below $\sim 500\text{K}$ causing the material to phase separate into $\text{Cs}_2\text{Fe}_4\text{Se}_5$, known as the 245 phase, and a minority Cs-site deficient and fully iron stoichiometric $\text{Cs}_x\text{Fe}_2\text{Se}_2$ phase (HT122). At slightly lower temperatures, the material undergoes another transition with the Fe spins of the main 245 phase ordering into an exotic checkerboard-type magnetic structure with a large magnetic moment. The minority LT122 phase is reported to either remain nonmagnetic or to become magnetic below $\sim 200\text{K}$. At temperatures below $\sim 30\text{K}$, the magnetic material becomes superconducting and the two states appear to coexist. Neutron and x-ray powder diffraction performed on ground crystals show that the average $I4/mmm$ structure of the minority phase is distinctly different from the high-temperature $I4/mmm$ parent structure. Moreover, single-crystal diffraction reveals the presence of discrete superlattice reflections that remove the degeneracy of the Cs sites in both the majority and minority phases and reduce their structural symmetries from body centered to primitive. Magnetization measurements performed in tandem with neutron single-crystal diffraction provide evidence that the minority phase is the host of superconductivity. Our results also reveal a superconducting dome in which the superconducting transition temperature varies as a function of the nominal valence of iron.

Synthesis and magnetic properties of the compound series $\text{La}_2\text{Zn}_{1-x}\text{Co}_x\text{IrO}_6$

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Recently 5d-metal oxides, such as iridates, have gained great interest. Due to their high degree of spin-orbit-coupling, they often have special physical properties like Mott-insulating-behavior.

Materials of the perovskite class have also been under intense research. Due to competing exchange interactions, there are several known materials in the perovskite-class that show interesting magnetic behavior, such as ferro- and antiferromagnetism, canted antiferromagnetism and spin-glass-behavior.

In iridates that adopt the perovskite-structure, the combination of these competing exchange interactions with the high degree of spin-orbit coupling, is expected to lead to unique physical phenomena.

The two literature-known compounds $\text{La}_2\text{ZnIrO}_6$ and $\text{La}_2\text{CoIrO}_6$ both show interesting magnetic behavior, ranging from canted antiferromagnetism of the Ir-sublattice in $\text{La}_2\text{ZnIrO}_6$ to a strong interaction between Ir- and Co-moments in $\text{La}_2\text{CoIrO}_6$.

In this study the intermediate compounds of the general formula $\text{La}_2\text{Zn}_{1-x}\text{Co}_x\text{IrO}_6$ were synthesized and, in order to gain a deeper understanding of the underlying exchange interactions, the evolution of magnetic properties throughout the series was investigated.

ACRT technique for the single crystal growth of the heavy-fermion compound YbRh_2Si_2

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In the heavy-fermion compound YbRh_2Si_2 the antiferromagnetic ordering below 70mK close to a quantum critical point is well-studied. Beneath the magnetic ordering a new phase transition was found recently at 2 mK. [1] It is necessary to prepare large and high-quality single crystals for studying the nature of this new phase transition. Besides the optimization of the single crystal growth it is important to investigate single crystals with different isotopes at this phase transition. Here, we report the crystal growth YbRh_2Si_2 with the accelerated crucible rotation technique (ACRT). ACRT shows for other compounds, e.g. YAG (yttrium aluminium garnet, $\text{Y}_3\text{Al}_5\text{O}_{12}$), that this technique can reduce flux impurities and enhance the yield of large crystals. We also report the attempt to receive metallic isotopes of ytterbium with metallothermic reduction. Crystals with different isotopes of silicon and ytterbium can be used for NMR measurements to investigate the underlying phenomena of quantum criticality in more detail.

[1] Schuberth et al. Science **351**, 485 (2016).

**oral session II: role of stoichiometry and ordering
(chair: A. Erb)**

09:00-09:45	Dharmalingam Prabhakaran (invited talk) "Floating Zone Growth – Challenges"
09:45-10:30	Stephen Wilson (invited talk) "Exploring the physical properties of a model correlated electron cathode material"
10:30-11:00	coffee break

Floating Zone Growth – Challenges

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Control of the oxidation state in transition-metal oxide compounds is important for studies of their magnetic properties. Usually it can be achieved by varying the partial pressure of oxygen, but for some materials which are thermodynamically unstable in ambient conditions, such as stoichiometric La_2NiO_4 , the crystal can be grown in a slight excess of oxygen and then the as-grown crystal annealed under a reduced atmosphere to achieve the stoichiometric composition. This is a key problem which I shall explore in this talk.

Another major challenge is the control of the evaporation rate. This can normally be done by applying a high pressure which stabilizes the growth. For example, in Na_xCoO_2 , Na_2O tends to evaporate strongly, and so by applying a high pressure and adding an excess of Na_2O the stoichiometry is retained. I will discuss this problem and show how the choice of pressure is critical for this approach.

Finally, site mixing and disorder is a very common problem in crystal growth. For example, some pyrochlore compounds can undergo dramatic changes in their magnetic properties due to this type of defect. I will discuss the effect of growth conditions on the resulting physical properties of some crystals.

Exploring the physical properties of a model correlated electron cathode material

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In the expanded search for alternative cathode materials within the realm of functional oxides, a number of strongly correlated electron materials are being explored as battery components. One model Na-based system in this realm is the layered compound Na_xMnO_2 ; a system with incredibly rich magnetic and structural properties of interest to both condensed matter physicists and materials scientists. In this talk, I will discuss some of our group's recent efforts exploring the fundamental magnetic and structural properties of this material and how crystal growth presents an exciting way forward in controlling its physical properties.

**oral session III: Intermetallics
(chair: W. Löser)**

11:00-11:45	Andrej Prokofiev (invited talk) "Floating zone growth of rare earth containing clathrates"
11:45-12:05	Ahmad Omar "Towards a novel half-metallic ferromagnet in the $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$ Heusler compounds"
12:05-12:25	Katharina Weber "Growing single crystals of peritectic YFe_4Ge_2"
12:25-12:45	Georg Benka "UHV-compatible preparation chain for high-purity single crystals of transition metal and rare earth compounds"
12:45-02:15	lunch at mensa

Floating zone growth of rare earth containing clathrates

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Type-I clathrates possess extremely low thermal conductivities, a property that makes them promising materials for thermoelectric applications. They are guest-host systems in which a large electropositive atom like Ba or alkali metals fills oversized polyhedral cavities in a covalently bound Si, Ge, or Sn framework. It is the interaction of the vibration mode of the guest atom (rattling) with the delocalized vibrations of the framework that results in the anomalously low thermal conductivity. The incorporation of cerium (Ce) into one such clathrate, the type-I clathrate $\text{Ba}_8\text{Au}_6\text{Si}_{40}$, has recently been shown to lead to a drastic enhancement of the thermopower, another property determining the thermoelectric efficiency [1]. This incorporation appeared to be feasible only via a crystal growth process implying the crystallization of the clathrate phase from an off-stoichiometric melt with an excess of Ce and Au. The developed floating zone technique was realized in a mirror furnace. The technique was now applied to clathrates containing other rare earth elements (RE). We discuss the mechanism of RE incorporation based on the trends in the clathrate phase composition along the RE element range. Our investigation reveals that the RE content is mainly governed by two factors, the residual cage space and the electron balance in the sense of the Zintl concept [2]. The thermoelectric and magnetic properties of some RE clathrates are discussed.

[1] A. Prokofiev, A. Sidorenko, K. Hradil, M. Ikeda, R. Svagera, M. Waas, H. Winkler, K. Neumaier, and S. Paschen. Thermopower enhancement by encapsulating cerium in clathrate cages. *Nature Mat.* **12** 1096-1101 (2013)

[2] S.C. Sevov. Zintl phases. In *Intermetallic Compounds, Principles and Practice: Progress*; Westbrook, J. H., Freisher, R. L., Eds.; John Wiley & Sons. Ltd.: Chichester, England, 2002; 113-132.

Towards a novel half-metallic ferromagnet in the $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$ Heusler compounds

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$\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$ Heusler compounds are predicted to show half-metallic ferromagnetism along the whole series, making them quite promising for application in spintronics. Unfortunately, the predicted properties have not yet been experimentally realized. We first show that the bulk polycrystalline samples in the series suffer from incongruent melting and are therefore chemically inhomogeneous. Furthermore, though Floating Zone growth of the selected compositions in the series, we shed light on a previously unreported low-temperature phase transformation via spinodal decomposition. Thus, almost all anomalous data in literature, both in bulk as well as thin films, could be reconciled.

In order to study the extent of the region of immiscibility, the phase-space in ternary Co_2CrAl was explored in terms of temperature and composition. The annealing experiments at different temperatures show that the secondary phase is stable till high temperatures and it is not possible to avoid it through thermal treatments. On the other hand, Floating Zone growth of off-stoichiometric compositions in Co_2CrAl clearly demonstrate that we tend to move out of the solid state miscibility gap as the Cr content is reduced against Al and a finally phase-pure sample was obtained.

The strategy for avoiding the phase transformation by optimizing the composition was applied to the $\text{Co}_2\text{Cr}_{0.6}\text{Fe}_{0.4}\text{Al}$ composition. Phase-pure sample was obtained using Floating Zone growth of the off-stoichiometric $\text{Co}_2\text{Cr}_{0.4}\text{Fe}_{0.4}\text{Al}_{1.2}$ composition. Band structure calculations show that the half-metallic ferromagnetism is still retained in the optimized composition. The magnetization and specific heat data also fit to theory, which makes the material quite promising as a novel half-metallic ferromagnet.

Growing single crystals of peritectic YFe_4Ge_2

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The intermetallic compound series AFe_4X_2 ($\text{A} = \text{Y}, \text{Lu}, \text{Zr}$; $\text{X} = \text{Si}, \text{Ge}$) presents a rare case of magnetic frustrated metallic systems. Our previous studies evidence the AFe_4X_2 family to cover the whole regime from frustrated antiferromagnetic (AFM) order up to the quantum critical point separating the frustrated AFM ground state from the paramagnetic ground state.

The synthesis is quite challenging as these compounds are strongly peritectic. So far, we have synthesised polycrystals of all compounds with a good sample quality. Now we are aiming to grow single crystals, which would allow studying the anisotropy of the magnetic and transport properties and especially detailed neutron studies to determine the magnetic structure and the magnetic excitations of the AFe_4X_2 compounds.

In my talk I will present the first attempts to grow single crystals of YFe_4Ge_2 in a mirror furnace. We have started the single crystal growth with YFe_4Ge_2 as it is less peritectic than the other AFe_4X_2 compounds. YFe_4Ge_2 is strongly frustrated with a $\theta_{\text{CW}}/T_{\text{N}}$ ratio of 2.5 and therefore is a good candidate to study frustration effects in itinerant systems.

UHV-compatible preparation chain for high-purity single crystals of transition metal and rare earth compounds

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The preparation of large high-purity single crystals is an important prerequisite for advances in solid state physics. We report the design of a single crystal preparation chain for intermetallic compounds under ultra-high vacuum compatible conditions. All furnaces are all-metal sealed, bakeable, and may be filled with high-purity argon gas, additionally purified by point-of-use gas purifiers. In particular, we report that optical float-zoning represents a powerful technique that combines decisive advantages, e.g., being crucible-free and allowing to address complex metallurgical phase diagrams via a travelling solvent approach. Using this preparation chain, we have successfully grown over 100 large single crystals of various intermetallic compounds, notably transition metal monosilicides, Heusler compounds, and various rare-earth systems. Important aspects of the preparation chain will be illustrated for the case of selected heavy fermion materials providing important bench markers.

**oral session IV: Ruddlesden Popper phases
and other perovskite related materials
(chair: K. Conder)**

02:15-03:00	Frank Lichtenberg (invited talk) „Melt-grown synthesis and structural and physical properties of $A_nB_nO_{3n+2} = ABO_x$ type materials and other perovskite-related layered oxides“
03:00-03:45	John Mitchell (invited talk) “Charge Stripes in Quasi-Two-Dimensional Trilayer Nickelate $La_4Ni_3O_8$”
03:45-04:00	Paul Sass “Ideas and future requirements for FZ technique”
04:00-04:30	coffee break

Melt-grown synthesis and structural and physical properties of $A_nB_nO_{3n+2} = ABO_x$ type materials and other perovskite-related layered oxides

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At the beginning some mirror furnaces and their special features will be presented. Also special components and concepts like pressing dies made of magnesia stabilized zirconia, the design and preparation of seed and feed rods, and sample holders made of Macor or yttria stabilized zirconia will be presented. In the next part perovskite-related layered oxides of the type $A_nB_nO_{3n+2}$, $A_{j+1}B_jO_{3j+1}$, $A'A_{k-1}B_kO_{3k+1}$, and $A_mB_{m-1}O_{3m}$ will be introduced. Some of these oxides such as $La_6Ti_4Fe_2O_{20}$ ($n = 6$), $Sr_5Nb_5O_{17}$ ($n = 5$), Sr_2RuO_4 ($j = 1$), $BaCa_2Nb_3O_{10}$ ($k = 3$), and $Sr_6Nb_5O_{18}$ ($m = 6$) can be prepared in crystalline form by floating zone melting and display often interesting physical and / or structural properties. Pictures of various crystalline oxides will be shown. Oxides of the type $A_nB_nO_{3n+2}$ are known for $n = 2 \dots 7$. They emerge from the 3D perovskite structure ABO_3 by a cut along its [110] direction and a subsequent insertion of additional oxygen. They are known for $B = Ti, Nb$ or Ta and the B site can be partly occupied by other elements such as Fe . Oxides of the type $A_nB_nO_{3n+2}$ comprise the highest- T_c ferroelectrics like $La_4Ti_4O_{14} = La_2Ti_2O_7$ ($n = 4$) with $T_c = 1770$ K and quasi-1D metals such as $Sr_5Nb_5O_{17}$ ($n = 5$) where the conduction electrons are embedded in a ferroelectric-like environment. It will be outlined why oxides of the type $A_nB_nO_{3n+2}$ might have a potential to create new multiferroics and superconductors.

Charge Stripes in Quasi-Two-Dimensional Trilayer Nickelate $\text{La}_4\text{Ni}_3\text{O}_8$

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The quasi-two-dimensional nickelate $\text{La}_4\text{Ni}_3\text{O}_8$ (La-438) phase consists of trilayer networks of square planar Ni ions, formally assigned as Ni^{1+} and Ni^{2+} in a 2:1 ratio. While previous studies on polycrystalline samples have identified a 105 K phase transition with a pronounced electronic and magnetic response but weak lattice character, no consensus on the origin of this transition has been reached. Here we show using synchrotron x-ray diffraction on high- $p\text{O}_2$ floating-zone grown single crystals that this transition is driven by a real space ordering of charge into a quasi-2D charge stripe ground state. The charge stripe superlattice propagation vector, $q=(\frac{2}{3}, 0, 1)$, corresponds with that found in the related 1/3-hole doped single layer Ruddlesden-Popper nickelate, $\text{La}_{5/3}\text{Sr}_{1/3}\text{NiO}_4$ (LSNO- $\frac{1}{3}$, $\text{Ni}^{2.33+}$) with orientation at 45° to the Ni-O bonds. Like LSNO- $\frac{1}{3}$, the charge stripes in La-438 are weakly correlated along the c axis to form a staggered *ABAB* stacking that minimizes the Coulomb repulsion among the stripes. Surprisingly, however, we find that the charge stripes within each trilayer of La-438 are stacked *in phase* from one layer to the next, at odds with any simple Coulomb repulsion argument.

Ideas and future requirements for FZ technique

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This contribution is dedicated to the discussion on future developments of the floating zone technique. – "What are the requirements and desires toward modern FZ instrumentation".

oral session V: novel materials I
(chair: S. Wurmehl)

09:00-09:45	Ryan C. Morrow (invited talk) "Superexchange Interactions in Double Perovskite Osmates"
09:45-10:30	Anna Isaeva (invited talk) "Crystal growth of new topological insulators in bismuth-halide and related systems"
10:30-11:00	coffee break

Superexchange Interactions in Double Perovskite Osmates

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Double perovskites containing rock salt ordered 3d and 4d/5d cations have been intensely studied for their wide range of technologically relevant properties. Design of functional materials in the insulating state, where magnetic properties are dictated by superexchange interactions, remains challenging however due to the poorly understood competition between numerous potential exchange pathways. In this work, a number of insulating double perovskite osmates, A_2BOsO_6 ($A = \text{Sr, Ca, La}$; $B = \text{Cr, Fe, Co, Ni}$) have been chosen and studied using magnetometry, specific heat, XMCD, and neutron powder diffraction techniques in order to systematically probe the effects of electronic configuration and bonding geometry on the magnetic ground state. It is concluded that the magnetic ground state is controlled by a tunable competition between short range and long range superexchange interactions which are sensitive to electronic configuration and bonding geometry.

Crystal growth of new topological insulators in bismuth-halide and related systems

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Topological insulators (TI) are a new class of materials with peculiar surface properties that open new prospects for spin transport. These bulk semiconductors host metallic states at their surfaces that are immune to backscattering [1] due to the specific symmetries of the band-structure and could thus transmit information without dissipation. Topological insulators and related materials are envisioned as promising candidates for innovative data storage and quantum bits. Since 2009 the outmost explored pool of TI materials has been limited to Bi_2Te_3 and related materials [2]; therefore a task of finding new candidates is of great importance.

The present contribution reports some highlights of our quest for new topological materials among bismuth-rich halides. Employing the concept of "confined metals" [3] we have established rough guidelines toward the directed search of new topological insulators based on crystal-structure features. This approach has by now yielded two 3D weak topological insulators ($\text{Bi}_{14}\text{Rh}_3\text{I}_9$ [4–6], Bi_2TeI [7]) and a 3D strong topological insulator, $\beta\text{-Bi}_4\text{I}_4$ [8], which electronic structure is in proximity of both the weak 3D TI phase and the trivial insulator phase. These bulk materials are built by two different 2D TI fragments: a decorated honeycomb intermetallic layer that resembles graphene and a bismuth bilayer, which is a building unit of the elemental bismuth structure.

Special focus is laid on optimization of the single-crystal growth methods for the above mentioned compounds. In order to observe and tackle surface properties directly with spectroscopic methods, large crystals with well-defined, atomically smooth surfaces are a necessary prerequisite.

[1] M.Z. Hasan, C. L. Kane. *Colloquium: Topological insulators*. Rev. Mod. Phys. **82** (2010), 3045.

[2] Y. Ando. *Topological insulator materials*. J. Phys. Soc. Jpn. **82** (2013), 102001.

[3] A. Isaeva, B. Rasche, M. Ruck. *Bismuth-based candidates for topological insulators: Chemistry beyond Bi_2Te_3* . Phys. Stat. Solidi RRL, 1–2 (2013), 39.

[4] B. Rasche, A. Isaeva, M. Ruck, S. Borisenko, V. Zabolotnyy et al. *Stacked topological insulator built from bismuth-based graphene sheet analogues*. Nat. Mater. **12** (2013), 422.

[5] B. Rasche, A. Isaeva, W. Van den Broek, M. Kaiser, et al. *Crystal Growth and Real Structure Effects of the First Weak 3D Stacked Topological Insulator $\text{Bi}_{14}\text{Rh}_3\text{I}_9$* . Chem. Mater. **25** (2013), 2359.

[6] C. Pauly, B. Rasche, M. Liebmann, M. Pratzner, et al. *Subnanometre-wide electron channels protected by topology*, Nat. Phys. **11** (2015), 338.

[7] I.P. Rusinov, T.V. Menshchikova, A. Isaeva, et al. *Mirror-symmetry protected non-TRIM surface state in the weak topological insulator Bi_2TeI* . Sci. Rep. **6** (2016), 20734.

- [8] G. Autès, A. Isaeva, L. Moreschini, J. C. Johannsen, A. Pisoni, et al. *Topological Insulator in Bismuth Iodide β -Bi₄I₄*. **Nat. Mater.** 15 (2016) 154.

oral session VI: novel materials II
(chair: A. Isaeva)

11:00-11:45	Binghai Yan (invited talk) "Topological surface states and chiral magneto-transport in TaAs-type of Weyl"
11:45-12.30	Seunghyun Khim (invited talk) "A new Type-II Weyl semi-metal candidate TaIrTe₄"

Topological surface states and chiral magneto-transport in TaAs-type of Weyl semimetals

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The Weyl semimetal (WSM) is new topological matter that is a 3D analogue of graphene. Recent discovery of WSM materials in TaAs-family of compounds has triggered tremendous interest to explore very exotic properties of those systems. In this talk, I will introduce our recent theoretical and experimental progress, which includes the surface Fermi arcs and the magneto-transport that is due to the chiral anomaly effect.

A new Type-II Weyl semi-metal candidate TaIrTe_4

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Orthorhombic ternary compound TaIrTe_4 has been predicted to be a type-II Weyl semi-metal. Here we report magnetotransport and magnetic quantum oscillations studies of TaIrTe_4 . The resistivity follows a $B^{1.5}$ -dependence up to 70 T without saturation similar to WTe_2 . The angular dependent de Haas-van Alphen oscillations detect two hole and two electron pockets. The sizes of the observed pockets are in a good agreement with the *ab initio* calculation with the Fermi level shifted by 30 meV. It gives an estimation that the Weyl nodes locate 50 meV above the Fermi level in the pristine TaIrTe_4 . It makes TaIrTe_4 a promising candidate for realizing a topological bulk state via slight tuning (doping or external pressure pressure) bringing the Weyl points to the Fermi level.