

# **European C-MetAC**

*European Integrated Center for  
the Development of New Metallic Alloys and  
Compounds*

***European C-MetAC Days 2021  
December 6 – 9, 2021  
(online)***

## ***Program***

**Schedule**

**Monday, December 6, 2021**

13:00	M. Konkel and M. Wencka: <i>Workshop Equality and diversity in material science</i>
17:00	J. Ledieu, Nancy: <i>Welcome note</i>
<i>Chair person: Peter Gille, Munich</i>	
17:15	H. Schlich, MaTecK GmbH: <i>Metal single crystal growth: Examples and challenges in the development of special crystals and their applications</i>
17:45	M. Armbrüster, Chemnitz: <i>Hunting ideal functional materials for applications in corrosive environments</i>

**Tuesday, December 7, 2021**

<i>Chair person: Ana Smontara, Zagreb</i>	
9:00	S. Penner, Innsbruck: <i>Steering the Catalytic Properties of Intermetallic Compounds and Alloys in Reforming Reactions by Controlled in Situ Decomposition and Self-Activation</i>
9:30	M. Majewicz, Wrocław: <i>Possible Lifshitz point in the magnetic phase diagram of UNi<sub>2</sub>Si<sub>2</sub> single crystals</i>
9:50	J. Juraszek, Wrocław: <i>Destruction of a sign-changing order parameter by artificial atomic defects in multiband superconductor PrOs<sub>4</sub>Sb<sub>12</sub></i>
10:10	I. Mandal, Krakow: <i>Correlated Insulators in Twisted Bilayer Graphene</i>
10:30	break
<i>Chair person: Silke Böhler-Paschen, Vienna</i>	
11:00	P. Popčević, Zagreb: <i>Interaction of magnetic and electronic subsystems in Co intercalated 2H-NbS<sub>2</sub> seen by different probes</i>
11:20	S. Sekh, Krakow: <i>Circular dichroism as a probe for band topology in chiral semimetals</i>
11:40	J.-M. Hübner, Dresden and Lund: <i>The Borosilicide Rb<sub>8</sub>B<sub>8</sub>Si<sub>38</sub> with a Clathrate-I type structure: high-pressure synthesis, cage adaption and properties</i>
12:00	lunch
<i>Chair person: Magdalena Wencka, Poznan and Ljubljana</i>	
13:30	N. Kanas, Novi Sad: <i>Heterostructuring - an effective way to boost zT of CaMnO<sub>3</sub>-based composites</i>
13:50	M. Uland, Chemnitz: <i>Chemical potential as guide in material development</i>
14:10	I. Antonyshyn, Dresden: <i>Isostructural M<sub>2</sub>Pt {M=Al, Ga, In, Sn}: structure - chemical properties - electrocatalysis</i>
14:30	O. Shedwick, Liverpool: <i>Analysis of the surface structure of a Ga<sub>3</sub>Ni<sub>2</sub> binary alloy using LEED &amp; STM</i>

14:50	break
<i>Chair person: Janez Dolinšek, Ljubljana</i>	
15:20	A. Jelen, Ljubljana: <i>Structure and microstructure of Sc-Hf-Nb-Ta-Ti-Zr refractory high-entropy alloys</i>
15:40	A. Gačnik, Ljubljana: <i>Superconductivity of Sc-Hf-Nb-Ta-Ti-Zr refractory high-entropy alloys</i>
16:00	P. Koželj, Ljubljana: <i>Magnetism in the magnetically concentrated, randomly disordered and frustrated CoCrFeMnNi HEA</i>
16:20	T. Seyller, Chemnitz: <i>Deposition of CrCoFeNi thin films by magnetron sputtering</i>
17:00 – 19:00	<i>Poster session</i>

**Wednesday, December 8, 2021**

<i>Chair person: Iryna Antonyshyn, Dresden</i>	
9:00	C. Goyhenex, Strasbourg: <i>Atomistic approach of the o-Al<sub>13</sub>Co<sub>4</sub> quasicrystalline approximant: point defects and surfaces</i>
9:30	O. Tiryaki, Chemnitz: <i>Investigating well-defined ZnPd/ZnO catalysts in methanol steam reforming</i>
9:50	M. Kotsch, Dresden: <i>Bell-Like [Gas] clusters in Sr<sub>3</sub>Li<sub>5</sub>Gas</i>
10:10	L. Rößner, Chemnitz: <i>Electrochemical investigations on intermetallic compounds</i>
10:30	break
<i>Chair person: Yuri Grin, Dresden</i>	
11:00	Elise Pachoud, Grenoble: <i>Crystal growth at the Néel Institute</i>
11:20	J. Smietanska, Krakow: <i>Looking at the modulated structure of pathogenesis-related protein (Hyp-1) complex with ANS within the higher dimensional superspace approach</i>
11:40	L. Agnarelli, Dresden: <i>Mg<sub>3</sub>Pt<sub>2</sub>: Anionic Chains in a Eu<sub>3</sub>Ga<sub>2</sub>-Type Structure</i>
12:00	lunch
13:30	R. Cardoso-Gil, Dresden: <i>Ga<sub>3</sub>Ir: a simple but complex material</i>
13:50	E. Gaudry, Nancy: <i>Two-dimensional metal structures revealed by evolutionary computations: Pb/Al<sub>13</sub>Co<sub>4</sub>(100) as a case study</i>
14:10	I. Buganski, Krakow: <i>The atomic model of the Tsai-type quasicrystal with AKNt rhombohedral units</i>
14:30	N. Saadi, Liverpool : <i>Compression behaviours of a 3D-printed quasicrystal</i>
14:50	break

*Chair person: Marc de Boissieu, Grenoble*

15:20	E. Svanidze, Dresden: <i>Compounds with mercury - complexity two ways</i>
15:40	C. Ruano M, Nancy: <i>2D OQC approximants in reduced SrTiO<sub>3</sub> grown on Pt(111)/Al<sub>2</sub>O<sub>3</sub>(0001)</i>
16:00	C.M.N. Kumar, Zagreb: <i>Structural investigation of super-ionic Cu<sub>2-x</sub>Se</i>
16:20	G. de Laitre, Grenoble: <i>Dynamical properties of the incommensurately modulated Rb<sub>2</sub>ZnCl<sub>4</sub> phase</i>
16:40	E. Pospíšilová, Bratislava: <i>Stable thin clathrate layers</i>
17:00	Concluding remarks

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***Thursday, December 9, 2021***

9:00	Science Board Meeting
10:30	break
11:00	Governing Board Meeting and General Assembly
12:20	lunch
13:30	Online announcement of the oral and poster prizes



***Abstracts  
of oral contributions***

***Metal single crystal growth: Examples and challenges in the development of special crystals and their applications***

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Crystals are one of the major pillars in the development and achievement of our modern technologies. This is most obvious for modern optics and the semiconductor industry. But also, the growth of metal single crystals is a key factor in basic research as metallic crystals are used to investigate physical and chemical effects for better understanding.

This presentation will show the main growth methods for metals and their alloys and their pros and cons will be discussed. Furthermore, the growth activities of the MaTecK company will be presented. Several examples will point out that crystal growth is a highly interdisciplinary subject that requires expertise in physics, chemistry, materials science and engineering. In detail, the development of crystals for neutron monochromators (based on Cu and Fe), for superalloys (based on Ni), for electrical propulsion of satellites (based on La) and for other metal single crystals and their alloys will be discussed.

## ***Hunting ideal functional materials for applications in corrosive environments***

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In many cases functional materials for chemical and physical applications have to withstand corrosive conditions during use. This comprises e.g. sensorics or catalysis. Especially the latter requires breaking and forming chemical bonds on the surface – of the material as well as the reactants and products. For an ideal catalysts, the material changes are fully reversible during a catalytic cycle, thus keeping the material functional on the long-term.

The required stability can be ensure by our recently developed chemical potential guided development (CPGD) which combines the information on the chemical potential of the elements within intermetallic compounds and the one of the corrosive environment. With this starting point, stable intermetallic platform materials<sup>[1]</sup> can be selected where each platform offers different electronic and structural properties.<sup>[2]</sup> The last step of the approach is to fine-tune electronic and geometric properties of the best platform materials by isostructural substitution with elements from the same period or the same group, respectively.<sup>[3,4]</sup>

Our approach enables the quick and directed development of functional materials in heterogeneous (electro)catalysis and beyond, circumventing laborous trial-and-error battles, which are often used in catalyst development.

### References

- [1] L. Röbner, et al. ACS Appl. Mater. Inter. 13, **2021**, 23616.
- [2] R. Zerdoumi, et al. Z.Anorg.Allg. Chem. 10.1002/zaac.202100171.
- [3] O. Matselko, et al. J. Phys. Chem. C 122, **2018**, 21891.
- [4] R. Zerdoumi, et al. ACS Appl. Energy Mater., accepted.

***Steering the Catalytic Properties of Intermetallic Compounds and Alloys in Reforming Reactions by Controlled in Situ Decomposition and Self-Activation***

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Based on the increasing importance of intermetallic compounds and alloys in heterogeneous catalysis, we explore the possibilities of using selected intermetallic compounds and alloy structures and phases as catalyst precursors to prepare highly active and CO<sub>2</sub>-selective methanol steam reforming (MSR) as well as dry reforming of methane (DRM) catalyst entities by controlled in situ decomposition and self-activation. The exemplary discussed examples (Cu<sub>51</sub>Zr<sub>14</sub>, CuZn, Pd<sub>2</sub>Zr, GaPd<sub>2</sub>, Cu<sub>2</sub>In, ZnPd, and InPd) show both the advantages and pitfalls of this approach and how the concept can be generalized to encompass a wider set of intermetallic compounds and alloy structures. Despite the common feature of all systems being the more or less pronounced decomposition of the intermetallic compound surface and bulk structure and the in situ formation of much more complex catalyst entities, differences arise due to the oxidation propensity and general thermodynamic stability of the chosen intermetallic compound/alloy and their constituents. The metastability and intrinsic reactivity of the evolving oxide polymorph introduced upon decomposition and the surface and bulk reactivity of carbon, governed by the nature of the metal/intermetallic compound-oxide interfacial sites, are of equal importance. Structural and chemical rearrangements, dictating the catalytic performance of the resulting entity, are present in the form of a complete destruction of the intermetallic compound bulk structure (Cu<sub>51</sub>Zr<sub>14</sub>) and the formation of an metal/oxide (Cu<sub>51</sub>Zr<sub>14</sub>, InPd) or intermetallic compound/oxide (ZnPd, Cu<sub>2</sub>In, CuZn) interface or the intertransformation of intermetallic compounds with varying composition (Pd<sub>2</sub>Zr) before the formation of Pd/ZrO<sub>2</sub>. In this talk, the prerequisites to obtain a leading theme for pronounced CO<sub>2</sub> selectivity and high activity will be reviewed. Special focus will be put on raising awareness of the intrinsic properties of the discussed catalyst systems that need to be controlled to obtain catalytically prospective materials. The use of model systems to bridge the material's gap in catalysis will also be highlighted for selected examples.

***Possible Lifshitz point in the magnetic phase diagram of UNi<sub>2</sub>Si<sub>2</sub> single crystals***

<sup>1</sup>\*M. Majewicz, <sup>1</sup>M. Szlawska, <sup>1</sup>D. Kaczorowski

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The ternary silicide UNi<sub>2</sub>Si<sub>2</sub> shows complex magnetic properties. In zero magnetic field, it undergoes a series of subsequent magnetic phase transitions from paramagnetic (PM) to incommensurate spin-density-wave (ICSDW) to antiferromagnetic (AF), and eventually ferrimagnetic (UAF) states. The external magnetic field causes metamagnetic transitions and stabilizes the UAF state. In high magnetic fields, the PM, ICSDW and UAF phases meet at a single point that may bear features of bicritical Lifshitz point (LP), which is a critical behaviour strikingly different from any other.

With the main aim to verify that LP hypothesis, we have undertaken comprehensive reinvestigation on high-quality single crystals of UNi<sub>2</sub>Si<sub>2</sub>. Our magnetization, electrical resistivity and heat capacity measurements confirmed the existence of multiple magnetic phases, and the tendency to mearing the PM-ICLSW and ICLSW-UAF phase boundaries. However, we failed to observe LP up to 14 T, the highest magnetic field accessible in our laboratory. Therefore, further study of the compound in even stronger magnetic fields is indispensable.

This work was supported by the National Science Centre of Poland grant no. 2018/31/D/ST3/03295.

***Destruction of a sign-changing order parameter by artificial atomic defects in multiband superconductor PrOs<sub>4</sub>Sb<sub>12</sub>***

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Chiral superconductivity is a long-sought unconventional state of matter that spontaneously breaks time-reversal symmetry through the development of Cooper pairing with finite angular momentum. Chiral superconductivity is a type of topological state which provides a natural platform for realizing Majorana edge modes being central to various proposals for quantum computation. However, despite intensive theoretical studies and huge experimental efforts, no material has been proven definitively to be a chiral superconductor.

The heavy-fermion and multiband superconductor PrOs<sub>4</sub>Sb<sub>12</sub>, for which a  $\mu$ SR study [1] and polar Kerr effect measurements [2] showed evidence of broken time-reversal symmetry spontaneously developing below the critical temperature  $T_c \simeq 1.85$  K, is a leading candidate to display chiral superconductivity. Based on measurements of the temperature dependence of the lower critical field  $H_{c1}(T)$ , we have recently proposed a multiband and multisymmetric scenario, in which a superconducting condensate is composed of a sign-changing smaller gap and a large isotropic s-wave gap [3].

To develop a detailed understanding of multicomponent superconductivity in PrOs<sub>4</sub>Sb<sub>12</sub>, we have extended measurements of  $H_{c1}(T)$  down to temperatures as low as 7 mK utilizing a 2DEG Hall magnetometry. We observe a sudden increase in  $H_{c1}(T)$  deep in a superconducting state, indicative of a rare case of two nearly decoupled bands. Furthermore, a non-saturating and concave behaviour of  $H_{c1}(T)$  below about 0.45 K clearly points at a sign-changing symmetry of the smaller gap. Equally remarkable is a high sensitivity of this characteristic to electron irradiation. Indeed, a concentration of artificial

atomic defects as small as a few 0.1% results in both a saturation of  $H_{c1}(T)$  at  $T < 0.15$  K and a strong suppression of the anomalous enhancement below  $\approx 0.25T_c$ , consistent with a destruction of an unconventional order parameter due to the smaller gap. In addition to this, theoretical description of possible symmetries of the smaller gap as well as results of a comparative study on the two-band isotropic s-wave homologue  $\text{LaRu}_4\text{As}_{12}$  will be discussed in the context of a putative chiral spin-triplet pairing state in  $\text{PrOs}_4\text{Sb}_{12}$  [4].

**References:**

- [1] [1] Y. Aoki et al., Time-Reversal Symmetry-Breaking Superconductivity in Heavy-Fermion  $\text{PrOs}_4\text{Sb}_{12}$  Detected by Muon-Spin Relaxation. *Phys. Rev. Lett.* **91**, 067003 (2003).
- [2] [2] E. M. Levenson-Falk et al., Polar Kerr Effect from Time-Reversal Symmetry Breaking in the Heavy-Fermion Superconductor  $\text{PrOs}_4\text{Sb}_{12}$ . *Phys. Rev. Lett.* **120**, 187004 (2018).
- [3] [3] J. Juraszek et al., Symmetry of Order Parameters in Multiband Superconductors  $\text{LaRu}_4\text{As}_{12}$  and  $\text{PrOs}_4\text{Sb}_{12}$  Probed by Local Magnetization Measurements. *Phys. Rev. Lett.* **124**, 027001 (2020).
- [4] [4] V. Kozii et al., Three-dimensional Majorana fermions in chiral superconductors. *Sci. Adv.* **2**, e1601835 (2016).

## ***Correlated Insulators in Twisted Bilayer Graphene***

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Recently, moiré superlattices in 2d van der Waals heterostructures have been found to exhibit properties analogous to the high- $T_c$  cuprates, namely, Mott insulating states and unconventional superconductivity. Examples include magic-angle twisted bilayer graphene and transition metal dichalcogenides. These being (chemically) simpler / cleaner systems compared to the transition metal oxide superconductors, have emerged as new experimental systems for studying strongly correlated phases, allowing higher degrees of experimental control. Experiments on twisted graphene bilayers, where the top layer is rotated with respect to the one below, have displayed insulating behavior when the moiré bands are partially filled. I will elaborate on our recent calculations to find the static charge configurations in these phases, and to estimate the excitation gaps.



***Interaction of magnetic and electronic subsystems in Co intercalated 2H-NbS<sub>2</sub> seen by different probes***

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Co<sub>1/3</sub>NbS<sub>2</sub> is a quasi 2D system where magnetic Co ions are positioned on triangular lattice in van der Waals gaps in-between metallic NbS<sub>2</sub> layers. The coexistence of metallic and magnetic degrees of freedom coupled with reduced dimensionality and anticipated frustration render this compound battlefield of different interactions resulting in peculiar antiferromagnetic (AF) ground state below 28K. So far, this is the only system from its family where complete suppression of AF order under relatively low hydrostatic pressure of 1.7 GPa was reported [1]. Another curiosity of this system is enhancement of the c-axis electrical resistivity observed in AF ordered state, indicating spin-valve like mechanism [2]. Last but not the least, angle-resolved photoelectron spectroscopy (ARPES) of Co<sub>1/3</sub>NbS<sub>2</sub> demonstrates limitations of the rigid-band model, which was traditionally used to describe materials from the same family. The most intriguing departure corresponds to appearance of a shallow electronic band at Fermi level with enhanced effective mass [3]. This band cannot be identified with any DFT calculated feature, and it is possibly related to the resonance caused by strong electron correlations.

References:

- [1] [1] N. Barišić et al. Phys. Rev. B, **84** (2011) 075157
- [2] [2] P. Popčević et al. arXiv: 2003.08127
- [3] [3] P. Popčević, Y. Utsumi et al. submitted.

***Circular dichroism as a probe for band topology in chiral semimetals***

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Topological semimetals, characterized by a singular or line degeneracy in the 3D Brillouin zone (BZ), have shown several interesting transport properties over the years due to their band topology. Recent discovery of 'multifold semimetals' such as RhSi, CoSi shows multiple degeneracies in the BZ is also possible where two or more bands meet with non-zero Chern number. Such multifold degenerate points lead to higher monopole charges as they harbour higher-pseudospin excitations with no counterpart in high-energy physics. However, detecting the topological invariant experimentally can be a daunting task. In our work, we demonstrate that analyzing the optical response of a circular drive is an effective way to detect the topology of the lowest-energy Bloch band, as it can be connected to a frequency-dependent probing function. This response depends on the excitation rates induced on the filled band by the left- and right-circular drive, because of the geometrical properties of the Bloch bands. Our calculation reveals that the response is quantized for rotationally-invariant Hamiltonians when the frequency of the drive is above a critical value. We demonstrate this numerically by considering three kinds of semimetals with pseudospin values of  $1/2$ ,  $1$ , and  $3/2$ , respectively. We also investigate the role of tilt and anisotropy and find that although tilt does not have any effect on the response, the presence of anisotropy can drastically hamper the quantization. Our scheme thus provides an important methodology for designing future experiments to detect the topology of band structures.

***The Borosilicide  $Rb_8B_8Si_{38}$  with a Clathrate-I type structure: high-pressure synthesis, cage adaption and properties***

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Clathrate-I borosilicides  $M_{8-x}B_ySi_{46-y}$  ( $M = K, Rb, Cs$ ) with alkali metals form under high-pressure, high-temperature conditions [1-4]. In contrast to clathrate-I silicides featuring larger substitution atoms like transition metals, boron substitution affects the 16i position located on the body diagonal of the unit cell. Boron substitution leads to a pronounced contraction of the lattice compared to the binary clathrate-I silicides. Remarkably, the lattice parameter of  $Rb_8B_8Si_{38}$  in space group  $Pm\bar{3}n$  ( $a = 9.9583(1) \text{ \AA}$ ) is strikingly similar to that of  $K_7B_7Si_{39}$  [1], in which half of the potassium positions on the body diagonal are empty. The alternative description of the clathrate-I structure as sodalite filled by dodecahedral cages explains the framework adaption to the larger rubidium atoms.  $Rb_8B_8Si_{38}$  shows a high thermal and chemical stability. The compound is an electronically balanced Zintl phase according to the formula  $(Rb^+)_8(B^-)_8(Si^0)_{38}$  consistent with its diamagnetic and semiconducting behavior.

***Heterostructuring - an effective way to boost  $zT$  of  $\text{CaMnO}_3$ -based composites***

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The effect of micro- and hetero-structuring on the thermoelectric properties of  $\text{CaMnO}_3/\text{CaMn}_2\text{O}_4$  composites is presented. Single phase compositions with rock salt structure were synthesized in reducing atmosphere and subsequently densified by spark plasma sintering in vacuum. Annealing in air at 1340 °C between 1 and 24 hours activated redox exsolution which resulted in a variation in microstructure of materials with 10 and 15 vol%  $\text{CaMn}_2\text{O}_4$ , respectively. The nature of the  $\text{CaMnO}_{3-\delta}/\text{CaMn}_2\text{O}_4$  interface was analyzed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) followed by a theoretical approach based on density functional theory (DFT). The bulk materials were characterized with respect to electrical conductivity ( $\sigma$ ), thermal conductivity ( $\kappa$ ) and Seebeck coefficient ( $S$ ) at temperatures between 300 and 900 °C in air. Besides the electrical conductivity of 73  $\text{S}\cdot\text{cm}^{-1}$  at 900 °C obtained with CMO15%24h, the highest  $\sigma$  and lowest  $\kappa$  were obtained for composites with 10 vol%  $\text{CaMn}_2\text{O}_4$  (CMO10%8h), reaching 49  $\text{S}\cdot\text{cm}^{-1}$  at 900 °C and 0.56  $\text{W}\cdot\text{m}^{-1}\text{K}^{-1}$  at 700 °C, respectively. However, the highest  $zT$  was obtained for samples with 15 vol%  $\text{CaMn}_2\text{O}_4$  (CMO15%8h) reaching 0.11 at 800 and 900 °C, due to the enhanced power factor above 700 °C.

## ***Chemical potential as guide in material development***

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Over the past decades, a wealth of data on the physical and chemical properties of a vast suite of functional materials has been collected – however, less progress has been made in connecting the catalytic properties of the material to those of its constituent elements. Understanding these relationships could allow for the prediction of a material's properties prior to synthesis. The elucidation of these connections is of particular relevance in the matter of catalyst stability, where there is a growing desire to predict a given material's stability under reaction conditions without wasting time and resources on its development and testing.<sup>[1]</sup> A possible solution is directed material development as guided by a carefully chosen descriptor – a material property that correlates to a material's stability<sup>[2]</sup> – and, in this vein, we propose using chemical potential as such a descriptor. Chemical potential can be defined most simply as a measure of a material's capacity for change under a given set of conditions and thus can be used to predict a material's stability under reaction conditions.<sup>[3]</sup> In addition to encapsulating a whole host of other thermodynamic factors<sup>[4]</sup>, chemical potential is intrinsic to a material and independent of the reaction being investigated<sup>[5]</sup>, offering a clear advantage over other proposed descriptors such as the adsorption energies of key reaction intermediates<sup>[6]</sup>.

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***Isostructural M<sub>2</sub>Pt {M = Al, Ga, In, Sn}: structure - chemical properties - electrocatalysis***

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Isostructural M<sub>2</sub>Pt {M = Al, Ga, In, Sn} crystallize with anti-CaF<sub>2</sub> type of crystal structure [1] and possess strongly polar covalent interactions between M and Pt atoms. The variation of the constituent component M leads to the different shift of the Pt 4f core levels towards higher binding energies (XPS data), increasing with decreasing of the atomic radii of M. In addition to charge transfer effects, XPS shifts are influenced by the final-state screening due to the conduction electrons. As a result, the correlation of XPS shifts with number of Pt 5d electrons was drawn based on ELI-D analysis.

The M<sub>2</sub>Pt specimens were used as oxygen evolution reaction (OER) electrocatalyst materials in water splitting reaction [2]. The OER activity follows the trend In<sub>2</sub>Pt > Ga<sub>2</sub>Pt > Al<sub>2</sub>Pt, governed by nature of M and their leaching rates upon conditions of OER. Intermetallic compounds M<sub>2</sub>Pt act only as catalyst precursors for formation of catalytically active M<sub>x</sub>Pt<sub>1-x</sub> phase in near-surface region. The remnant M<sub>2</sub>Pt plays a role of current collector and provide the integrity of the bulk electrode. The compound Sn<sub>2</sub>Pt is inactive for OER due to the formation of passivating layer of SnO<sub>2</sub> on the surface and hindrance of electron transfer through it. In addition to comprehensive experimental characterization of materials before and after OER, the first-principle calculations were performed to shed a light onto the change of Pt electronic state during the leaching.

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***Analysis of the surface structure of a Ga<sub>3</sub>Ni<sub>2</sub> binary alloy using LEED & STM***

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Intermetallic compounds have been of interest in the field of catalysis for many years[1]. From their reaction specificity to being made from more inexpensive metals intermetallic compounds offer many new options in particular as replacements for rare earth catalyts. Ga<sub>3</sub>Ni<sub>2</sub> is a binary alloy that is used in the reduction of CO<sub>2</sub> into CO and methanol at atmospheric pressures[2].

As Ga<sub>3</sub>Ni<sub>2</sub> is used as a heterogeneous catalyst for the reduction of CO<sub>2</sub> understanding the surface of catalyst is important [3]. Using the surface probing techniques of LEED, Low Energy Electron Diffraction a process that uses the diffractions of electrons to probe the surface of the sample, and STM, Scanning Tunnelling Microscopy an experimental method used to image the surface in the sample by measuring the change in voltage as a tip moves across the surface. The (2, -1,0) surface of Ga<sub>3</sub>Ni<sub>2</sub> has undergone both LEED and STM then the results were compared with the model structure of the bulk crystal.

The preliminary results seem to indicate that 1x1 reconstruction is being seen primarily in the LEED data with the reconstruction also been seen in the FFT of the large terraces of the Ga<sub>3</sub>Ni<sub>2</sub> surface.

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## Structure and microstructure of Sc-Hf-Nb-Ta-Ti-Zr refractory high-entropy alloys

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We have investigated scandium (Sc)-containing Sc-Hf-Nb-Ta-Ti-Zr system of refractory high-entropy alloys (HEAs), with all elements in equiatomic concentrations.

Unlike the Hf-Nb-Ta-Ti-Zr parent HEAs, which possess a single-phase body-centered cubic (bcc) structure and quite homogeneous microstructure, the addition of Sc produces a two-phase structure in the Sc-Hf-Nb-Ta-Ti-Zr alloys, with one phase being body-centered cubic (bcc) and the other hexagonal close-packed (hcp). The hcp phase absorbs practically all Sc, whereas the bcc phase is identical to the bcc phase of the Hf-Nb-Ta-Ti-Zr parent system. Upon Sc addition, the microstructure becomes very inhomogeneous. Large bcc dendrites of sever 10 – 100  $\mu\text{m}$  dimension are homogeneous in the central parts (Fig. 1 a), but become a fine dispersion of sub-micron precipitates of the bcc and hcp phases close to the edges. The interdendritic regions are also similar fine dispersion of the two phases, with no larger ( $\mu\text{m}$ -size) hcp regions (Fig. 1 b).

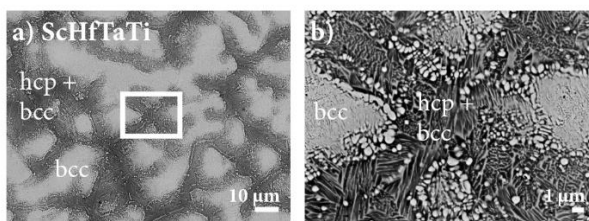


Fig. 1: BSE SEM images of a ScHfTaTi high-entropy alloy; a) low mag. image showing hcp + bcc (dark) and bcc (light) phases, with white rectangle indicating the enlarged area in b), showing fine dispersion of the two phases.



***Superconductivity of Sc-Hf-Nb-Ta-Ti-Zr refractory high-entropy alloys***

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In an attempt to enhance the physical-mechanical properties of the Hf-Nb-Ta-Ti-Zr refractory HEAs, we have employed additional element scandium. Its addition caused the formation of a highly inhomogeneous two-phase (bcc and hcp) structure. The hcp phase has absorbed practically all Sc, leaving the elemental composition of the remaining bcc phase identical to the bcc phase of the Hf-Nb-Ta-Ti-Zr parent system.

Heat capacity, magnetic susceptibility, and electrical resistivity measurements revealed similar superconducting properties to the bcc Hf-Nb-Ta-Ti-Zr parent alloys. The superconducting phase is a type II superconductor and BCS-like. The enormous chemical and structural disorder classify it as the Anderson "dirty" superconductor [1]. The main effect of Sc addition is to suppress superconductivity of the hcp phase fraction and to introduce higher chemical disorder in the superconducting bcc phase.

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***Magnetism in the magnetically concentrated, randomly disordered and frustrated CoCrFeMnNi HEA***

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In addition to the obvious complication of several different kinds of atoms, magnetism in high entropy alloys is also influenced by the micro- and nanostructure formed during sample synthesis and annealing. This contribution [1] will deal with a high-quality non-equiatomic CoCrFeMnNi synthesized via the Czochralski method, where these two difficulties have been removed via proper thermal treatment so that the sample is homogenous on the microscale (SEM elemental mapping) and without short-range ordering or chemical inhomogeneity on the nanoscale (APT, HAADS STEM and EELS).

The appeal of our HEA as an unusual magnetic system is that it is a severely concentrated and multielemental magnetic system (since all 5 elements are magnetic) which is a completely random solid solution with frustrated FM and AFM interactions. We have observed that the system undergoes a transition to a spin glass state at  $T_f \approx 20$  K. The broken ergodicity below  $T_f$  in CoCrFeMnNi was demonstrated via ZFC-FC magnetization splitting, the shift of the cusp in AC susceptibility measurements, the ultra-slow decay of thermoremanent magnetization and the thermal memory effect.

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***Deposition of CrCoFeNi thin films by magnetron sputtering***

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We report on the deposition of CrCoFeNi high entropy alloy (HEA) films by magnetron sputtering, which is a widely used technique for thin film deposition. In a first set of experiments, two type of sputter targets were produced by spark plasma sintering: a so-called alloy target from a homogeneous, equimolar CrCoFeNi HEA powder and a so-called blend target from an equimolar mixture of pure metal powders. Thin films were deposited by magnetron sputtering on Si(001) and stainless steel substrates. A characterization of the thin films using X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), X-ray fluorescence spectroscopy (XRF) and scanning electron microscopy (SEM) revealed negligible differences in composition and structure of the polycrystalline, cubic (fcc) HEA films prepared from the two different targets. This suggests that HEA films can be grown from considerably cheaper blend targets.

In a second set of experiments, thin films were grown on MgO(001) and Al<sub>2</sub>O<sub>3</sub>(0001) substrates using the alloy target. This resulted in (001) and (111) oriented, cubic CrCoFeNi films with very well ordered surfaces as demonstrated by low-energy electron diffraction. This opens a route towards future studies of the surface properties of HEAs without the need for growing bulk single crystals.

***Atomistic approach of the o-Al<sub>13</sub>Co<sub>4</sub> quasicrystalline approximant : point defects and surfaces***

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The Al<sub>13</sub>Co<sub>4</sub> intermetallic compound has attracted the attention of many research groups due to its unusual physical and chemical properties. A few examples include its strongly anisotropic magnetic and electronic transport behavior [1], its interesting catalytic performances towards hydrogenation reactions [2], as well as its unexpected wetting properties [3]. To understand these fascinating features, the determination of structure-properties relationships is crucial. This task is however challenging, since defects play a non negligible role in this compound [1,4]. Indeed accurate and reliable modelling of Al<sub>13</sub>Co<sub>4</sub> where structural complexity and local disorder are at play, requires large computational cells. The same holds for studies involving surfaces. In this talk, we will present a tight-binding atomistic approach based on the use of an N-body potential parameterized for the o-Al<sub>13</sub>Co<sub>4</sub> quasicrystalline approximant. We will show its ability to model this complex compound in the presence of atomic vacancies or surfaces thanks to the use of classical molecular dynamics simulations [5]. The importance of stress relaxation in vacancy formation will be highlighted through the presentation of a mapping of the local pressures in the bulk compound. Thanks to the many body character of the potential, the surfaces could be investigated which was not done before in atomistic studies of this complex phase. The results are compared to previous studies involving both DFT calculations and experiments [6]. Finally, preliminary investigations of the wetting of lead on the o-Al<sub>13</sub>Co<sub>4</sub>(100) surface, using classical molecular dynamics, will be also presented.

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## Investigating well-defined ZnPd/ZnO catalysts in methanol steam reforming

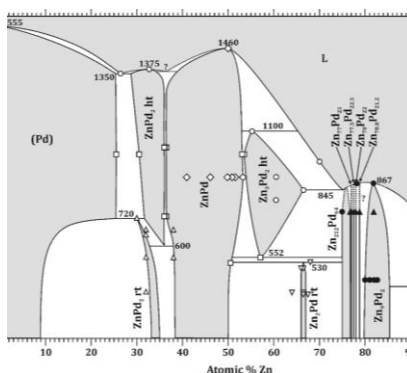
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ZnPd/ZnO catalysts are promising methanol steam reforming (MSR) catalysts, because they can produce lower CO containing hydrogen feeds for fuel cell applications, as compared to Cu-based catalysts. In addition, they have proven to have higher thermal stabilities. [1] Highly active and selective materials are Zn-rich compositions of ZnPd[2] (wide homogeneity range, Fig. 1), which determine the surface composition and thus also the oxidisability of the zinc on the surface. Due to the complexity



Pd-Zn phase diagram.[3]

of the supported materials, it is expedient to first examine the changes to unsupported Zn-Pd samples and then to increase the complexity on the material side. The unsupported ZnPd compounds need to be examined operando regarding their dynamic material changes in a reactive atmosphere. This contribution will give preliminary insights into sample preparation and characterization in the pristine state.

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**Bell-Like [Ga<sub>5</sub>] clusters in Sr<sub>3</sub>Li<sub>5</sub>Ga<sub>5</sub>**

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The unique bell-like [Ga<sub>5</sub>] cluster was first discovered by Fedorchuk et. al. in the compound Eu<sub>3</sub>Li<sub>5+x</sub>Ga<sub>5-x</sub> (x = 0.15).[1] The presence of *f* electrons in combination with the dual valency of europium however hindered the application of quantum chemical calculations in order to gain further insight into the bonding situation of this cluster. This problem however, can be circumvented by replacing europium with an alkaline-earth metal, in analogy to Ba<sub>3</sub>LiGa<sub>5</sub>. [2] In the present case this was achieved through the utilization of strontium, resulting in the isostructural compound Sr<sub>3</sub>Li<sub>5</sub>Ga<sub>5</sub> (space group  $R\bar{3}m$ ,  $a = 9.6040(5)$  Å,  $c = 22.061(1)$  Å).

Identically to Eu<sub>3</sub>Li<sub>5+x</sub>Ga<sub>5-x</sub> the compound Sr<sub>3</sub>Li<sub>5</sub>Ga<sub>5</sub> can formally be counted as [Sr<sup>2+</sup>]<sub>3</sub>[Li<sup>1+</sup>]<sub>5</sub>[(1b)Ga<sup>4+</sup>]<sub>1</sub>[(3b)Ga<sup>2-</sup>]<sub>3</sub>[(4b)Ga<sup>1-</sup>]<sub>1</sub> according to the Zintl concept, whereas the combined analysis of electron density (ED) and electron localizability indicator (ELI-D) revealed a much more complex situation. In particular, it was found that the Ga-Ga contacts forming the triangular base of the bell-like cluster have no interaction with each other, which leads to a different Zintl count, ([1b)Ga<sup>4+</sup>]<sub>4</sub>[(4b)Ga<sup>1-</sup>]<sub>1</sub>) requiring more electrons than provided. However if the partially bonding character of the lone pairs is considered,<sup>[3]</sup> it results in an electronically balanced scheme: [(1b)Ga<sup>2.5-</sup>]<sub>4</sub>[(4b)Ga<sup>1-</sup>]<sub>1</sub>. In combination with the [Sr<sub>6</sub>] polycation found in the structure, this indicates a reorganization tendency towards a Wade-like cluster anion with less electrons necessary for its stabilization.

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**Electrochemical investigations on intermetallic compounds**

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To bridge the gap of sample morphologies between solid-state chemistry (unsupported bulk samples, thin-films, powders) and applied electrocatalysis (carbon or oxide supported nano-particles), a unified approach for testing well characterized un-supported materials is developed. The approach allows to evaluate the intrinsic catalytic properties of numerous samples in a short period of time.

The approach is based on using intermetallic compounds as platform materials, providing a reproducible sample surface. This can be used as a reference-state for further electrocatalytic- and physical characterization techniques (Fig. 1). The approach has been successfully applied for the hydrogen evolution reaction (HER) on intermetallic Mo-Ni compounds [1] as well as an high entropy alloy composed of Al, Fe, Co, Cu and Ni. Additionally, the methanol oxidation reaction (MOR) was investigated on intermetallic compounds within Pd<sub>2</sub>(Ga/In/Sn/Zn) (CoSi<sub>2</sub> type of crystal structure) [2,3] and Pt(Sn/Bi/Pb) (NiAs type of crystal structure).

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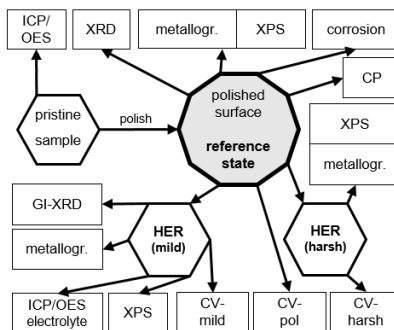


Figure 1 Exemplary analysis strategy utilizing the reproducible reference state.



***Crystal growth at the Néel Institute***

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***Looking at the modulated structure of pathogenesis-related protein (Hyp-1) complex with ANS within the higher dimensional superspace approach***

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Newly discovered, and still uncommon, modulated crystal structure in organic systems require a deeper investigation. No exact and detailed solution of such systems has not been done up-to-date. One possibility is to use an approximation of commensurate modulation which enables constructing a supercell, extending to the case, where translational symmetry (periodicity) is recovered, and simplify the analysis [1]. An assumption of commensurateness of the modulation is, however, questionable and rather unverifiable.

The goal of our studies was to use a novel, original statistical method of structural modeling which enables a refinement based on the average unit cell with (commensurate or incommensurate) modulation without unclear assumption of commensurateness and supercell approach. The main concept of the statistical method is to express structure in terms of the statistical distribution of atomic positions concerning the periodic reference lattice with lattice constant related to characteristic length-scale present in the structure. The average unit cell, defined as a probability distribution, constructed for periodic crystal is the same as the unit cell. The statistical approach was successfully used for the description of not only periodic crystals or quasicrystals, as well as it can be expanded on modulated structures as well as aperiodic structures with singular continuous components in the diffraction pattern [2].

Our model system is a pathogenesis-related protein (Hyp-1) complex with fluorescent probe 8-anilino-1-naphthalene sulfonate (ANS), which is a unique example of a macromolecular system with the modulated crystal structure. Previous studies have shown that Hyp-1/ANS complexes are tetartohedral twinned and crystallized in an asymmetric unit cell containing a repetitive motif of four protein molecules arranged with 7-fold noncrystallographic

repetition along the c axis of the C2 space group. Assumption of commensurate structure modulation demanded description of structure in the highly expanded unit cell with 28 unique protein molecules inside [3]. The Hyp-1/ANS structure was solved by molecular replacement and refined using maximum-likelihood targets with reliability factors  $R_{\text{work}}/R_{\text{free}}$  of 22.3/27.8%, respectively.

Our approach involved re-integration of raw data, development of the original software in Matlab environment and multidimensional analysis used to build the structure model and perform the refinement for significant improvement of results. The problem of incorporating disorder in the form of phonons into structural analysis was also carried out traditionally by Debye-Waller factor.

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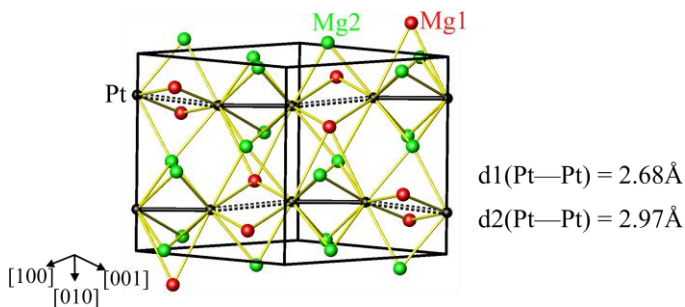
***Mg<sub>3</sub>Pt<sub>2</sub>: Anionic Chains in a Eu<sub>3</sub>Ga<sub>2</sub>-Type Structure***

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During the investigation of the Mg-Pt system, a new intermetallic compound was identified, Mg<sub>3</sub>Pt<sub>2</sub>. The title compound can be obtained through a direct reaction between the components or using the spark-plasma synthesis with MgH<sub>2</sub> and PtCl<sub>2</sub> as reagents. Mg<sub>3</sub>Pt<sub>2</sub> crystallizes in the monoclinic space group *C2/c* with  $a=7.2096(3)$  Å,  $b=7.1912(4)$  Å,  $c=6.8977(3)$  Å, and  $\beta=106.072(3)$  ° and is isotypic to Eu<sub>3</sub>Ga<sub>2</sub>. The striking feature of the crystal structure is anionic parallel chains of Pt atoms, with alternating Pt-Pt distances, stabilized by a complex multicentre interaction involving Pt and Mg species (Figure 1).



**Figure 1.** Parallel Pt metal chains with Mg atoms acting as bridges between two parallel chains.  $d1$  (blackline), shorter distances between the Pt atoms in the chain;  $d2$  (dashed black line), longer distance between the Pt atoms in the chain.

### ***Ga<sub>3</sub>Ir: a simple but complex material***

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The intermetallic compounds with the composition T<sup>(8)</sup>Tr<sub>3</sub> (T = group 8 transition metals and Tr: gallium or indium; crystal structure FeGa<sub>3</sub>-type, space group P4<sub>2</sub>/mnm) are semiconductors. On the other hand, isostructural T<sup>(9)</sup>Ga<sub>3</sub> compounds with T = group 9 transition metals should show metallic behavior. However, theoretical calculations predicted a narrow band-gap of ~0.15–0.07 eV for IrGa<sub>3</sub>.

ht-Ga<sub>3</sub>Ir is a high-temperature phase crystalizing also in the FeGa<sub>3</sub> type of structure. Pure ht-Ga<sub>3</sub>Ir was synthesized from the elements by quenching from 1173 K and characterized by powder and single-crystal XRD, metallography, WDXS and thermal analysis. The thermoelectric characterization of ht-Ga<sub>3</sub>Ir was performed and the temperature-dependent electrical resistivity measurements evidenced a semiconductor behavior, with a band-gap of 30 meV. From the single-crystal X-ray diffraction data, a model for the real crystal structure of ht-Ga<sub>3</sub>Ir is derived by the split-position approach and confirmed by atomic-resolution TEM study [1].

The thermal analysis of ht-Ga<sub>3</sub>Ir shows its peritectic formation at 974°C and peritectoid decomposition at 799°C. Additionally, a yet unknown reaction at 530 °C was observed and interpreted as the peritectoid formation of the low temperature phase lt-Ga<sub>3</sub>Ir. The crystal structure of lt-Ga<sub>3</sub>Ir (sample annealed and quenched from 400 °C) was solved using 3D-ED electron diffraction data (space group Pnma, crystal structure Fe<sub>3</sub>C-type), optimized by quantum-mechanical techniques and refined from the X-ray powder diffraction data [2].

References:

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**Two-dimensional metal structures revealed by evolutionary computations:  
Pb/Al<sub>13</sub>Co<sub>4</sub>(100) as a case study**

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We have combined extensive Density Functional Theory calculations with an evolutionary algorithm to investigate possible structural models for two-dimensional (2D) Pb films supported on the Al<sub>13</sub>Co<sub>4</sub>(100) quasicrystal approximant. The minimization of the total energy with the constraint of maximizing the atomic density in the layer leads to 2D atomic arrangement with pentagonal motifs, reflecting the symmetry of the substrate. Our findings show that the 2D Pb structure can be interpreted as a stable structure, with 16 Pb atoms in the surface cell, in good agreement with the measured coverage and scanning tunnelling microscopy images. Alternatively, a metastable 15-atom 2D film also fits with the experimental observations. This study opens a route towards the prediction of supported complex 2D films [1].

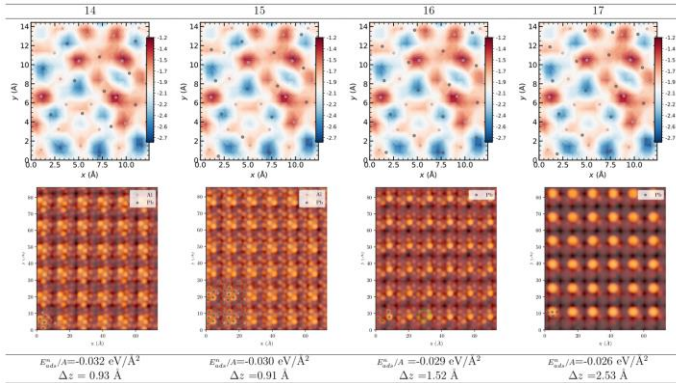


Fig. 1 : Adsorption energies, structures and simulated STM (scanning tunneling microscopy) images for 2D Pb-films with different atomic densities on Al<sub>13</sub>Co<sub>4</sub>(100).

References:

- [1] F. Brix and E. Gaudry , Two-dimensional metal structures revealed by evolutionary computations: Pb/Al<sub>13</sub>Co<sub>4</sub>(100) as a case study, submitted

***The atomic model of the Tsai-type quasicrystal with AKNt rhombohedral units***

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The atomic structure model of CdYb [1] quasicrystal became a universal standard for all icosahedral quasicrystals with Tsai clusters. The model is praised for its geometrical simplicity and chemical order. Atoms cluster in simple shapes like icosahedron, triacontehedron, etc. Clusters are linked via rhombic faces of triacontahedron along 2-fold axis (b-linkage) and interpenetrate along 3-fold axis (c-linkage). The unavoidable gaps between clusters are filled with rhombohedral units decorated according to the simple-decoration scheme.

Recently, a structural model of ZnMgTm was developed [2]. The model was founded on different principia than the CdYb model. The unique decoration of rhombohedra in Amman-Kramer-Neri tiling (AKNt) was found and exploited for structural study. When the model was interpreted for atomic clusters, the linkage along 5-fold axis was found. Not only that. The additional linkage discards the necessity of having gap-filling atoms. Even though i-ZnMgTm is a Bergman quasicrystal, it brings questions regarding CdYb model. Can the Tsai quasicrystal be solved in the same manner? In this work, the atomic structure of CdYb quasicrystal is solved using the AKNt and the structural features arising as a consequence of the model are discussed.

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- [2] Buganski, I., et al., Acta Cryst. A76 (2020), 180-196

## ***Compression behaviours of a 3D-printed quasicrystal***

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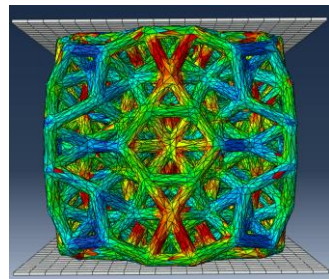
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For many years lattice type structures have been researched for their mechanical properties with the goal of producing lightweight materials that possess high strength and high stiffness. Additive manufacturing has been used as a way to rapidly prototype these mostly periodic or amorphous structures for mechanical testing. In this study, the mechanical properties of macro-scale aperiodic structures in compression are investigated.

3D models are manufactured using Stereolithography (Form 3, Formlabs, USA) a 3D-printing technology that uses a laser to cure a photosensitive resin layer-by-layer producing a part directly from a CAD model. Quasi-static compression tests are conducted on a 3D printed Tsai-type approximant model to study the mechanical properties of this aperiodic structure and in later stages, assess the energy absorption.

Using Finite Element Analysis (FEA), computer simulations of the lattice under stress are created to compare the theoretical compression behaviours of the aperiodic structure to the 3D-printed experimental findings. With control of the relative density, 3D printed quasicrystal structures could be compared to their periodic counterparts with respect to properties such as specific stiffness, strength and energy absorption.



*Figure 2 Contour plot of a deformed Tsai-type QC in Abaqus CAE.*



***Compounds with mercury – complexity two ways***

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Mercury, in both elemental form and as part of compounds and amalgams has played an important role in solid-state chemistry and condensed matter physics. However, much care must be taken both during synthesis as well as during characterization of this peculiar element and its compounds – from toxicity concerns to high chemical reactivity – these systems pose several experimental challenges. In this talk I will showcase that, nonetheless, mercury-based materials offer unique crystallographic motifs and, as a result, peculiar physical properties. In particular, I will concentrate on the uranium-mercury binary compounds which have so far been under investigated. By looking at the evolution of crystallographic complexity across the series that contains four binary compounds, I will discuss how atomic arrangement particularities affect the resultant ground states. I will also highlight some of the experimental advances we have been developing in order to synthesize and characterize uranium-mercury compounds, as they pose several handling difficulties as a result of extreme air-and moisture-sensitivity.

## 2D OQC approximants in reduced SrTiO<sub>3</sub> grown on Pt(111)/Al<sub>2</sub>O<sub>3</sub>(0001)

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We report an all-thin film staging approach to investigate the SrTiO<sub>3</sub>/Pt(111)/Al<sub>2</sub>O<sub>3</sub>(0001) system, where three different oxide quasicrystal (OQC) approximants were observed by means of low energy electron diffraction and scanning tunneling microscope. High-resolution images show bright protrusions located at the node of the different tilings constructed with the same basic square, triangle and 30° rhombus tiles possessing a common edge length of about 6.7 Å.

Depending on the preparation conditions, we identified a giant square-like approximant, consisting in 72 elements; a large hexagonal approximant, consisting in 29 elements; and the  $\sigma$ -approximant, consisting in only 5 elements.

The structural and electronic properties of the phases were investigated by means of density functional theory (DFT). Simulated microscopy images were also obtained from a model identifying the bright protrusions as Sr atoms, providing an excellent agreement with the experimental observations. Charge transfer is found to occurs at the interface, from most electropositive elements (Sr, Ti) to most electronegative ones (Pt and O), influencing the rumpling and the adhesion energy of the oxide films.

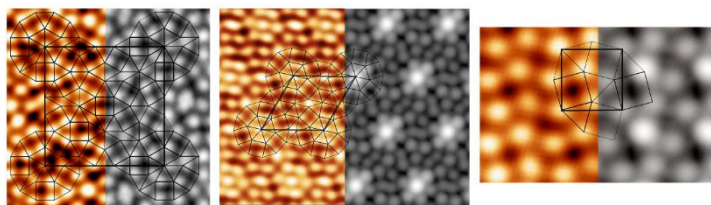


Figure 1. Comparison between the experimental (orange) and calculated (gray) STM images for the square (left), the hexagonal (middle) and the  $\sigma$ -approximant (right).

*The ideal unit cells decorated with square, triangle and rhombus tiling elements are highlighted as well.*

### ***Structural investigation of super-ionic Cu<sub>2-x</sub>Se***

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Materials that exhibit the super-ionic behavior present an extremely promising perspective for replacing liquid electrolytes in batteries with solid-state ion conductors and could revolutionize super-capacitors, fuel cells, and solid-state batteries [1]. Fast ion transport in many of such materials is supported by a disordered, ‘liquid-like’ sub-lattice of cations mobile within a rigid anionic sub-lattice. Transition metal chalcogenide (TMC) Cu<sub>2-x</sub>Se has attracted much attention recently due to its super-ionic behavior [2]. In Cu<sub>2-x</sub>Se with liquid-like copper lattice within the FCC selenium lattice, there is an indication of the super-ionic phase surviving down to room temperatures (and even below) making it an extremely promising material for technological applications. The phase diagram of Cu<sub>2-x</sub>Se has been intensively investigated previously, but data differ across literature [3, 4]. Here we present results of our synchrotron x-ray diffraction studies which show direct correlation between structure and ionic behavior of Cu<sub>2-x</sub>Se in a wide temperature range.

References:

- [1] Hu L. et al, *Nanomaterials* **10**, 302 (2020).
- [2] Liu, H. et al., *Nature Materials* **11**. 422–425 (2012).
- [3] Glazov, V. M. et al., *Inorganic Materials* **36**, 641-652 (2000).
- [4] Tonejc, A. et al., *J. Matter. Sci.* **15**, 3090-3094 (1980).

***Dynamical properties of the incommensurately modulated Rb<sub>2</sub>ZnCl<sub>4</sub> phase***

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Aperiodic crystals are long-range ordered crystals that lack periodicity. Although their structure is well described, their dynamics are more debated. In particular, phason modes have been experimentally observed in few incommensurately modulated phases.

The Rb<sub>2</sub>ZnCl<sub>4</sub> phase displays several transitions. Above T<sub>i</sub>=303K the HT phase is described as a crystal structure of space group P<sub>mcn</sub> where ZnCl<sub>4</sub> tetrahedrons have disordered orientations. From T<sub>i</sub>=303K, down to T<sub>C</sub>=195K, orientations of these tetrahedrons get incommensurately modulated along the c axis with an increasing anharmonicity. Below T<sub>C</sub>, the modulation gets locked-in, the c cell parameter is then tripled. We probed the dynamics of this material through inelastic neutron scattering for T between 140K and 350K.

At 140K TA phonons associated to the satellite reflections are indistinguishable from others. However their intensity decreases abnormally with increasing T, while a growing quasi-elastic signal localized around satellite positions expands. This signal remains localized in the HT phase despite the prevailing disorder. We discuss its relation with the modulation and its phasonic nature.

***Stable thin clathrate layers***

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Energies per atom and surface energies of pure Sn, Ge and Si clathrate free-standing nanofilms as a function of coverage (number of atoms per unit area of the slab) are evaluated in wide range of slab thicknesses from 1 to 10 ML (units of (111)-diamond monolayers). The stability of clathrate nanofilms is assessed by comparison with metallic beta and gamma phase slabs of Sn as well as with several distinct reconstructions of (111)-terminated diamond slabs including 3x3, 7x7 DAS (Dimer + Adatom + Stacking Fault) reconstructions which are the principal competitors to Ge and Si clathrates. In the case of Sn and Ge, the stability region of the clathrate thin films with reconstructed surface is clearly recognizable.

***Abstracts  
of poster contributions***



**Structural and chemical properties of UHV-prepared CeRu<sub>4</sub>Sn<sub>6</sub> (001) and (010) surfaces**

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<sup>2</sup>X. Lyan, <sup>2</sup>D. A. Zocco, <sup>2</sup>A. Prokofiev and <sup>2</sup>S. Paschen

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Recently, it has been theoretically predicted that CeRu<sub>4</sub>Sn<sub>6</sub>, a heavy fermion system, belongs to a new class of strongly correlated topological materials [1]. The calculated electronic structure exhibits Weyl fermions, opening a new direction of research in condensed matter physics. A way to demonstrate the presence of such quasiparticles is to use angle-resolved photoemission spectroscopy (ARPES) in combination with other techniques. ARPES is a surface sensitive tool hence requiring clean and atomically flat surfaces under ultra-high vacuum. A common way to experimentally proceed is to use in situ cleaved single crystals. However, cleavage might lead to different surface layers with different composition and high rugosity directly impacting band structure and measurement reproducibility. Moreover, many large samples are necessary. An alternative way is to prepare surfaces by Ar<sup>+</sup> sputtering and annealing cycles. Evidently, the main benefit is that a single crystal with controlled surface composition and orientation can be reused at will for reliable investigations. In this work, we investigate the morphology and chemical composition of CeRu<sub>4</sub>Sn<sub>6</sub> surfaces with either (001) or (010) orientation cleaned by sputtering and annealing cycles as a function of annealing temperature (T<sub>a</sub>). Using low-energy electron diffraction, scanning tunneling microscopy and X-ray photoemission, we show that the surface exhibits flat terraces and 3D islands with sharp facets and that the Sn content at the surface varies with T<sub>a</sub>. Surface energies of possible bulk truncated models have been computed based on density functional theory calculations. Preliminary ARPES results will be presented and discussed.

The work in Vienna was supported by the Austrian Science Fund (I4047, P29279).

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P-2

## Adsorption energies determined by machine learning on the low-index $Al_{13}Co_4$ complex surfaces

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Complex phases and quasicrystal-related compounds have recently emerged as promising catalysts. Understanding the structure-catalytic properties relationships requires the determination of the adsorption energies in a first step. The most efficient methods to draw the adsorption energy landscape of surfaces are based on Density Functional Theory (DFT). These approaches are however quite time consuming when complex surfaces are considered. Here, we investigate how machine learning approaches can accurately provide adsorption energies from a few DFT estimates. Our study focus on the adsorption properties of atomic H, O and Pb on quasicrystalline  $Al_{13}Co_4$  low-index surfaces. For instance, we see on figure (1) that the root mean square error (RMSE), representing the precision of the prediction, increase with the mass of the atom adsorbed by the compound.

Finally, the accuracy and the transferability of the different models are discussed and compared to the existing literature.

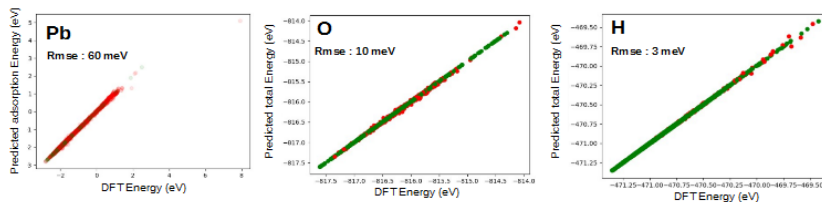


Figure 3: Predicted energy compared to DFT energy for an atom of Pb, O, H on the  $Al_{13}Co_4(100)$ . We put a criteria for the precision of 10 meV, the dots in green are the predicted values below the criteria.





***Supported (ultra)-thin films: how strong is the impact of the substrate to enforce a specific structure?***

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The crystal growth of a film over a substrate is a fascinating field, due to the complexity of the parameters involved. Crystalline, amorphous or polycrystalline structures can emerge, induced by key factors such as the interplay between the relative strengths of adsorbate-adsorbate and adsorbate-substrate interactions, the system's temperature, the complexity of the substrate surface, and the flux of incoming species [1]. Quasicrystal surfaces have been found as perfect template structures for the growth of single-element pseudomorphic thin films. But quasicrystalline order can also emerge on periodic metals, as recently discovered by Forster et al. [2]. In this work, we focus on two types of model structures to investigate interfaces with a quasiperiodic character. First, a quasicrystalline approximant oxide deposited over a periodic metallic substrate ( $\text{BaTiO}_3/\text{Pt}(111)$ ) [3], and second, a thin alumina phase (amorph and  $\theta$ ) deposited over a complex intermetallic substrate ( $\text{Al}_9\text{Co}_2/\text{Al}_2\text{O}_3$ ). Calculations based on Density Functional Theory are performed to determine the influence of the substrate (showing a short or larger periodicity) over different types of oxides films. As a preliminary result, the adhesive energy is stronger ( $-0.27 \text{ eV}/\text{\AA}^2$ ) in the  $\text{BaTiO}_3/\text{Pt}(111)$  system than in the  $\text{Al}_9\text{Co}_2/\text{Al}_2\text{O}_3$  ( $-0.11$  and  $-0.15 \text{ eV}/\text{\AA}^2$  for  $\theta$  and amorph, respectively). Further studies will aim to investigate the impact of other factors on the adhesion, such as the atomic density of the film or the charge transfer.

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- [3] Thiago Trevizam Dorini et al. In: Nanoscale 13.24 (2021), pp. 10771–10779. issn: 2040-3364, 2040-3372.



***Pd-In intermetallic nanoalloys stability:  
a DFT study of shape, size, and composition.***

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Nanoalloys combine finite size effects and alloy effects, significantly extending the range of nanomaterial properties. A crucial step for the control of these properties is to characterize structural and chemical arrangements.

Experiments have made impressive progress to synthesize and characterize nanoalloys of controlled size, morphology and composition. However, the precise chemical arrangement at the surface is still challenging to observe, meaning experiments often need simulations to refine their interpretations. It is particularly significant in catalysis since the catalytic properties depend on the atomic arrangements at the surface. Pd-In nanoalloys exhibit higher activity and selectivity than the monometallic Pd catalyst for selective acetylene hydrogenation but the performance of this catalyst depends on the composition<sup>1</sup>, PdIn surfaces present good catalytic properties for CO<sub>2</sub> hydrogenation to methanol<sup>2</sup>. Intermetallic systems such as Pd-In are well known to present a high enthalpy of formation in the bulk and no surface segregation. By reducing the system size, from alloy to nanoalloy, a lot of questions arise: Is chemical ordering conserved? What is the morphology of nanoalloys? Is there surface segregation?

We propose a DFT study of the stability of Pd-In nanoalloys as a function of size, shape and chemical arrangements to answer these questions. This is a crucial step before any investigation of catalytic properties.

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P-5

**Ammonia synthesis on the LaRuSi Electride Catalyst**<sup>1</sup>F. Brix, <sup>2</sup>G. Frapper and <sup>1,\*</sup>E. Gaudry

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Recently, transition metal electrides have attracted the attention of scientists as promising catalysts for ammonia synthesis. But very little is known about the atomic processes involved. In this work, extensive DFT calculations are performed to explore the detailed mechanism of ammonia synthesis catalyzed by LaRuSi, a typical electride catalyst. In sharp contrast to the recent proposal involving the high surface energy Ru-termination of LaRuSi(001), we show that an alternative reaction path on the most stable La-termination is more likely. Our study addresses the contrasted catalytic properties of the isostructural LaRuSi electride and CaRuSi non-electride compounds. It points the role of surface La atoms in the catalytic performances of LaRuSi, and shows that active sites are not necessarily transition metal atoms. Our findings open up future explorations of transition metal free catalysts for ammonia synthesis, active under mild conditions [1].

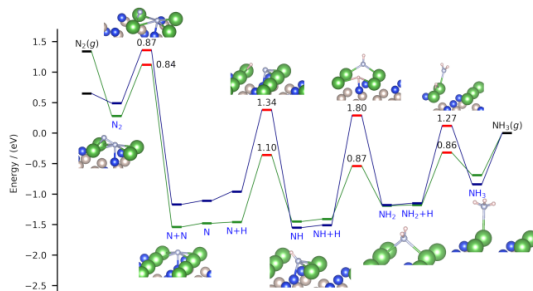


Fig.1 : Reaction energy diagram for ammonia synthesis on LaRuSi(001) and CaRuSi(001) surfaces (in blue and green, respectively).

## References:

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**P-6**

***De Haas-van Alphen oscillations in  $Zr_xHf_{1-x}SiS$***

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Among three-dimensional (3D) systems with non-trivial topological states, topological nodal-line (TNL) semimetals attract much attention due to their particularly interesting physics. In topological nodal-line semimetal Dirac band crossings occur along a line or form a loop in momentum space. Representatives of this type of material are ZrSiS and HfSiS. Since Zr and Hf are isovalent and of similar size,  $Zr_xHf_{1-x}SiS$  compound is stable for  $x \in [0,1]$ .

In this poster we present synthesis of  $Zr_xHf_{1-x}SiS$  monocrystals for various  $x$  and show De Haas-van Alphen quantum oscillations in magnetization for several directions of external field up to 7 T.

**P-7**

***Investigation of chemical order in  $Gd_{14}Au_xAl_{86-x}$  quasicrystal 1/1 approximants***

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Quasicrystals (QCs) exhibit crystallographically forbidden symmetries and aperiodic long range atomic order, whereas approximants of quasicrystals (ACs) possess conventional periodic crystal structures with similar chemical composition and local atom arrangements as their related QCs. For the past 40 years, there has been considerable interest in finding new QCs and ACs, and investigating their physical properties. The effect of chemical composition on magnetic behavior has been recently reported for ACs  $Gd_{14}Au_xAl_{86-x}$ . [1]. In particular it was found that with increasing Au concentration magnetism changes from spin glass behavior to FM to AFM. In order to better understand the underlying reasons for the observed magnetic properties in it was deemed necessary to determine the crystal structures of  $Gd_{14}Au_xAl_{86-x}$  1/1 ACs for a broader range of x. Therefore, high quality single crystals with different Au/Al ratio have been synthesized using the self-flux method. The phase purity of the samples have been confirmed by EDX and powder XRD techniques. The crystal structure was refined from single crystal XRD data. As a result, some atomic sites show strong chemical preference while others are resilient. The specifics of the chemical ordering phenomenon in  $Gd_{14}Au_xAl_{86-x}$  1/1 ACs will be discussed.

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**P-8**

***Design and fabrication of a micro-sample holder for thermopower measurement using photolithography***

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The application of the temperature gradient along the sample, which is at a uniform chemical potential, creates an energy imbalance per charge that eventually leads to charge diffusion from one side of the sample to the other. This leads to the generation of the electric potential difference. To a linear approximation, it is proportional to the applied temperature gradient, the Seebeck coefficient being the coefficient of proportionality. In general, it gives information about the topology of the Fermi surface, but is generally difficult to model.

The measurement of the Seebeck coefficient is also not an easy task. The main difficulty is to measure accurately the temperature difference along the sample. Normally, we measure it with a differential thermocouple consisting of three thin wires whose connections are electrically linked, for example by soldering or spot welding. To overcome these difficulties, we have developed a sample holder on a chip with low thermal conductivity. The chromel constantan thermocouple is deposited on it by a combination of a two-step process involving magnetron sputtering and micropatterning by photolithography. In this work we describe the fabrication process in detail.



***Investigation of CeRu<sub>4</sub>Sn<sub>6</sub> under hydrostatic pressure***

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The landscape of novel quantum phases in strongly correlated systems is expected to be further enriched in the presence of nontrivial electronic topology. A candidate material to explore this regime is the tetragonal, non-centrosymmetric Kondo semimetal CeRu<sub>4</sub>Sn<sub>6</sub>. Recent theoretical work predicted that it hosts Weyl points in its renormalized bandstructure near the Fermi level [1]. In addition, inelastic neutron scattering experiments revealed that CeRu<sub>4</sub>Sn<sub>6</sub> is quantum critical without tuning [2]. These results raise the interesting question of whether the Weyl-Kondo semimetal may be an emergent phase stabilized by quantum fluctuations. In this work we address this question by investigating the specific heat and magnetotransport properties of CeRu<sub>4</sub>Sn<sub>6</sub> single crystals under hydrostatic pressure. Our specific heat results suggest that applying pressure tunes CeRu<sub>4</sub>Sn<sub>6</sub> away from quantum criticality. At the same time, electrical transport indicates that a “background” Kondo-insulator gap is enlarged by pressure. We also study putative signatures of Weyl-Kondo physics.

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**P-10**

***Investigation of bulk ZnPd catalysts using  
high resolution electron microscopy***

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Methanol Steam Reforming (MSR) is an important reaction converting methanol into hydrogen ( $\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow 3 \text{H}_2 + \text{CO}_2$ ) holding promise for easy fuel handling in hydrogen based applications like fuel cells. ZnPd/ZnO nanoparticles prove to be promising MSR catalysts due to their high  $\text{CO}_2$  selectivity, stability and activity.<sup>1</sup> Their activity and selectivity depends very sensitively on their Zn/Pd ratio, even though the relevant intermetallic PdZn phase has a wide compositional existence range.<sup>2</sup> In order to elucidate the relationship between composition, microstructure, and catalytic performance, ZnPd samples with different composition were characterized using high resolution transmission electron microscopy (HRTEM) and energy dispersive X-ray spectroscopy (EDX). Furthermore, first identical location and in-situ experiments under MSR conditions are conducted to elucidate the microstructural changes of the ZnPd system under realistic operation conditions.

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**P-12**

***Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N<sub>x</sub> with isolated [Ga<sub>4</sub>] tetrahedra:  
synthesis, modifications and twinning***

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In the context of our recent work in the M–Li–Ga systems (M = Sr, Ba, Eu) with the aim of synthesizing compounds with isolated [Ga<sub>n</sub>] clusters [1,2], we have obtained Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N<sub>x</sub>, which is stabilized only by the presence of nitrogen. The synthesis was performed by using stoichiometric amounts of elemental Ba and Ga, excess of Li as flux for crystal growth and different amounts of Li<sub>3</sub>N as nitrogen source. The flux was subsequently removed by high-temperature centrifugation-aided filtration.

Two modifications are obtained. Whereas the hexagonal h-Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N<sub>x</sub> (space group P6<sub>3</sub>mc, a = 9.8495(5) Å, c = 6.8092(7) Å) is formed by nitrogen deficit, the orthorhombic o-Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N<sub>x</sub> (space group Pmnn, a = 9.82388(6) Å, b = 17.0474(1) Å, c = 6.84496(4) Å, (b/a)<sup>2</sup> = 3.011) is obtained if larger amounts of nitrogen are present. A series of experiments revealed that the critical amount of nitrogen needed for the transition from P6<sub>3</sub>mc to Pmnn modifications is approximately 10 % of the stoichiometric amount in Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N. The single-crystal investigation of o-Ba<sub>6</sub>Li<sub>8</sub>Ga<sub>8</sub>N<sub>x</sub> is hampered by twinning (three-domains).

The structures of both compounds are strikingly similar, only differing in the respective orientation of the isolated [Ga<sub>4</sub>] tetrahedra. The [Ba<sub>6</sub>] octahedra in both structures are interconnected into columns through face-sharing, and act as host for the N atoms resembling the Mn<sub>5</sub>Si<sub>3</sub> structure type arrangement. The formation of different [Ga<sub>n</sub>] clusters in binary and ternary gallides is discussed in dependence of valence electron concentration per Ga atoms and electronegativity of the constituent elements

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**P-13**

***Al<sub>2</sub>Cu(001) studied by photo electron spectroscopy 2.0***

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Intermetallic compounds have received interest because of their performance as catalysts in, e.g., hydrogenation reactions. However, compared to the enormous number of surface studies on pure metals and on alloys, there are considerably fewer studies on the surface properties of intermetallic compounds.

Recently, Al<sub>2</sub>Cu(001) showing a  $(2\sqrt{2}\times\sqrt{2})R45^\circ$  reconstruction was studied using low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) in combination with ab initio calculations [1]. The aim of our work is to further characterize the Al<sub>2</sub>Cu(001) surface by additional techniques, in particular X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). The poster will present and discuss first results of our work, focusing on surface composition and structure as well as electronic structure. We investigate the effects of surface preparation by sputtering and annealing on the stoichiometry obtained from XPS measurements and the formation of different surface reconstructions. Measurements of the electronic band structure are presented along the high-symmetry directions of the surface Brillouin zone and compared to LMTO calculations [2].

References:

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- [2] M. Armbrüster, PhD Thesis, TU Dresden (2004)

**P-14**

***Low temperature charge transport in  $WN_x$***

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We report low temperature electrical properties (resistivity, thermopower and magnetoresistance) of a transitional metal nitride (TMN) pelet. TMNs are interesting both because of their good mechanical properties, which make them suitable for design of new cutting tools, and because of their electrical properties, which predestine them for new electrode materials [1][2].

In our samples, nitride to metal ratio is suggested to be  $>1$  because of clear Mott-like resistance above 20K [3]. In  $<20K$  regime we observe change in resistivity.

The magnetoresistance is measured in a magnetic field directed both parallel and perpendicular to the current flow. In both cases, the magnetoresistance curves have a similar shape, typical for ferromagnets, while at the same time we observe no significant change in shape below and above 20 K.

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**Physical and structural properties of  $\text{Cu}_{2-x}\text{Se}$  across**

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$\text{Cu}_2\text{Se}$ , as a competitive thermoelectric material, has attracted much attention recently [1], mainly due to its large figure of merit (ZT), which is among highest for single crystalline compounds (1.5 at 1000K). This is predominantly associated with its superionic behavior in the high-temperature  $\beta$ -phase which also holds potential for applications in solid state batteries [2].

Although high temperature  $\beta$ -phase was extensively investigated, comprehensive insight of low temperature  $\alpha$  phase is still lacking. It reflects the complexity of the structural and phase relations. The transition temperature from  $\alpha$  phase to  $\beta$  phase considerably depend on  $x$  and mixed phase is between them [4]. We observe large temperature hysteresis probably related to the mechanism of this phase transition. The shape of hysteresis is strongly time dependent. Here we present detailed magnetotransport and thermoelectric properties of  $\text{Cu}_{2-x}\text{Se}$  at low temperatures complemented with structural and magnetic studies. They will allow us to understand mechanism of order-disorder phase transition in  $\text{Cu}_{2-x}\text{Se}$  subsystem which most probably lies behind wide temperature hysteresis observed in our results.

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