

ECMetAC Days 2023

# **BOOK OF ABSTRACTS**

27<sup>th</sup> – 30<sup>th</sup> November 2023

Kranjska Gora, Slovenia

Book of Abstracts

ECMetAC Days 2023, Kranjska Gora, Slovenia, 27<sup>th</sup> – 30<sup>th</sup> November 2023

Editors: Primož Koželj, Stanislav Vrtnik, Jože Luzar, Andreja Jelen

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Dear Colleagues,

We would like to welcome you to the ECMetAC Days 2023 conference, taking place in Hotel Kompas in Kranjska Gora, Slovenia from 27<sup>th</sup> to 30<sup>th</sup> November 2023. The conference is a continuation of the series ECMetAC Days, organized annually by a member institution of the European Integrated Center for the Development of Metallic Alloys & Compounds (ECMetAC, <https://www.ecmetac.eu/>). This year's ECMetAC Days is organized by the Jožef Stefan Institute (JSI, Ljubljana, Slovenia) and the Faculty of Mathematics and Physics of the University of Ljubljana (Ljubljana, Slovenia). JSI is the organizer of a conference from this series for the second time, after C-MAC Days 2013 (taking place before the name change from C-MAC to ECMetAC).

The topics of the conference series include formation, stability, synthesis, structural and chemical characterization, physical, chemical and mechanical properties, surfaces and thin films, catalysis, theory, applications and new frontiers in metallic materials. The topics are approached in a highly interdisciplinary manner and include mathematics, physics, chemistry, metallurgy and materials science.

Based on the submitted contributions, we can say that ECMetAC Days 2023 will provide an excellent opportunity to present and get acquainted with the latest results in the field of newly discovered metallic alloys and compounds. A broad range of materials will be discussed during the eight sessions of talks and one poster session – conventional crystalline intermetallics, complex metallic alloys, quasicrystals and their approximants, metallic glasses, high-entropy alloys, intermetallics for catalysis, correlated-electron systems, thermoelectrics, magnetocalorics and related materials.

We wish you a productive ECMetAC Days 2023 and a pleasant stay in the beautiful Alpine resort of Kranjska Gora!

Prof. Dr. Janez Dolinšek and the local organizing committee

Ljubljana, November 2023



## **Local Organizing Committee**

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Peter Mihor  
Dr. Jože Luzar  
Dr. Andreja Jelen  
Assist. Prof. Dr. Primož Koželj  
Assist. Prof. Dr. Stanislav Vrtnik  
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## ORGANIZING INSTITUTIONS



Jožef Stefan Institute, Ljubljana, Slovenia

University of *Ljubljana*  
Faculty of *Mathematics and Physics*





# Program



# Monday, 27<sup>th</sup> November

12:00 – 18:00 Registration

13:30 – 14:30 Lunch

## **Workshop (Magdalena Wencka):**

### ***Innovative Researcher: End-User Approach for Scientific Project Designing***

14:30 – 16:30 Workshop p. 23

16:30 – 17:00 Coffee break

17:00 – 18:30 Workshop p. 23

19:00 – 20:30 Get together party

# Tuesday, 28<sup>th</sup> November

8:50 – 9:00 Opening (**Magdalena Wencka, Julian Ledieu**)

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9:00 – 9:30 **Peter Gille** (LMU München) p. 27  
*Single crystal growth of  $In_7Pd_3$ : A case study*

9:30 – 9:50 **Ireneusz Bugański** (AGH Kraków) p. 28  
*The structural similarity between Tsai- and Bergman-type phases*

9:50 – 10:10 **Zbigniew Śniadecki** (IMP PAS Poznań) p. 29  
*The thermodynamic stability of the  $ThMn_{12}$ -type phase in new hard magnetic  $(Ce,Zr,Nd)Fe_{10}Si_2$  alloys*

10:10 – 10:30 **Nazar Zaremba** (MPI CPfS Dresden) p. 30  
*Searching for new uranium-based arsenides*

10:30 – 11:00 Coffee break

## Session 2 Chairperson: **Thomas Seyller**

11:00 – 11:20 **Oksana Karychort** (MPI CPfS Dresden) p. 32  
*New Samarium Iron Arsenide  $SmFe_5As_3$*

11:20 – 11:40 **Andrzej Krzysztof Musiał** (IMP PAS Poznań) p. 33  
*Prussian Blue Analog as a precursor for synthesizing of  $Ni(Fe, Co)$ -based nanoparticles*

11:40 – 12:00 **Woiciech Sas** (IP Zagreb) p. 34  
*Strategies of synthesizing Prussian blue analogs of mixed composition into reduced dimensionality systems*

12:00 – 12:20 **Andreja Jelen** (JSI Ljubljana) p. 35  
*Diverse microstructures of the magnetic high-entropy alloys*

12:20 – 12:40 **Ahowd Yousef Alfahad** (Uni-Liverpool) p. 36  
*Surface structure of  $In_3Ni_2$  intermetallic compound*

12:40 – 14:30 Lunch

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*Topological semimetals in strongly correlated systems*

15:00 – 15:20 **Julia Petrović** (JSI Ljubljana) p. 40  
*Kondo effect in  $Ce_xLaLuScY$  ( $x = 0.05-1.0$ ) high-entropy alloys*

15:20 – 15:40 **Anton Kabaši** (US Split) p. 41  
*Anisotropic thermal conductivity of hydrogen fuel cell catalyst films*

15:40 – 16:00 **Monika Kušter** (JSI Ljubljana) p. 42  
*Effect of Al-Cu-Fe quasicrystal particles on the reinforcement of a polymer-matrix composite: from mechanical to surface properties*

16:00 – 16:30 Coffee break

**Session 4** Chairperson: **Hem Raj Sharma**

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*Stability and electronic properties of two-dimensional oxide quasicrystal approximants*

16:50 – 17:10 **Vipin Kumar Singh** (IJL Nancy) p. 45  
*Transformation of two-dimensional quasicrystalline approximants into partially filled honeycomb lattices in reduced  $SrTiO_3$  thin films supported on  $Pt(111)/Al_2O_3(0001)$*

17:10 – 17:30 **Thomas Seyller** (CUT Chemnitz) p. 46  
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17:30 – 19:00 Poster session

19:00 Dinner

20:00 – 22:00 EB meeting

# Wednesday, 29<sup>th</sup> November

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9:30 – 9:50 **Wilfried Bajoun Mbajoun** (IJL Nancy) p. 52  
*C<sub>60</sub> adsorption on the (100) surface of Au-Si-Ho Tsai-type approximant*

9:50 – 10:10 **Émilie Gaudry** (IJL Nancy) p. 53  
*Structural, ordering, and magnetic properties of PtNi nanoalloys explored by density functional theory and stability descriptors*

10:10 – 10:30 **Pavol Priputen** (SUT Trnava) p. 55  
*Characterization of Co-Fe-Ni-Cu-based multi-principal element alloys*

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## Session 6 Chairperson: Marek Mihalkovič

11:00 – 11:20 **Janusz Tobała** (AGH Kraków) p. 56  
*Interplay of electronic structure and electrochemical efficiency in cathode materials for Li- and Na-ion batteries*

11:20 – 11:40 **Emil Babić** (FS UZ Zagreb) p. 57  
*Compositionally complex alloys: some insight from photoemission and magnetism*

11:40 – 12:00 **Federico Mazza** (VUT Vienna) p. 58  
*Scrutinizing the phonon Kondo effect in intermetallic clathrates*

12:00 – 12:20 **Marko Kuveždić** (FS UZ Zagreb) p. 59  
*Two parallel conducting channels in compositionally complex amorphous alloys of early and late transition metals*

12:20 – 12:40 **Primož Koželj** (JSI Ljubljana) p. 60  
*Magnetism in a nanostructured single-crystalline Al<sub>28</sub>Co<sub>20</sub>Cr<sub>11</sub>Fe<sub>15</sub>Ni<sub>26</sub> high-entropy alloy*

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15:40 – 16:00 **Kacper Jakub Pryga** (AGH Kraków) p. 66  
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16:50 – 17:10 **Jože Luzar** (JSI Ljubljana) p. 68  
 *$\text{AlCoFeNiCu}_x$  ( $x = 0.6\text{--}3.0$ ) and  $(\text{GaNi})_x\text{CoCrFe}$  ( $x = 0.4\text{--}1.6$ ) zero-magnetostriction magnetically soft high-entropy alloys for supersilent AC magnetic applications*

17:10 – 17:30 **Liam Chandler** (UL Liverpool) p. 69  
*Magnetic properties of quasiperiodic artificial spin-ice tilings fabricated with nanolithography*

17:30 – 17:50 **Pavol Noga** (SUT Trnava) p. 70  
*New ToF ERDA experimental setup at the Slovak University of Technology in Bratislava for the characterisation of hydrogen storage and battery materials*

17:50 – 18:00 Closing (**Janez Dolinšek, Julian Ledieu**)

19:00 Gala dinner

## Thursday, 30<sup>th</sup> November

8:30 – 10:15 Science Board meeting

10:15 – 10:45 Coffee break

10:45 – 12:30 Governing Board meeting and General Assembly

12:30 Lunch

## **List of posters**



# List of posters

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**Monday afternoon**

**27<sup>th</sup> November 2023**

**Workshop**





## Innovative Researcher: End-User Approach for Scientific Project Designing

M. Wencka

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Design Sprint (DS) is a methodology for quickly and effectively solving design problems. It draws on design thinking, i.e. creative design of solutions to problems, products and services, as well as other practical methods used in business. It is our wish to apply the DS approach also in science to make researchers more sensitive to end-users needs at the earliest stages of materials and products design and production. The DS process consists of five following stages that use design thinking to reduce risk and negative consequences when bringing a new project/product: understand (definition of the project goal), sketch (sketching of new ideas), decide (selecting the best solution), prototype (raw version of the project) and test (collecting opinions, further works on the product). The DS allows for a fast and cheap prototyping of ideas and their subsequent implementation. This workshop is dedicated to scientists whose research covers all levels of the Technology Readiness Levels (TRLs) starting from observations of basing principles (basic research levels TRL1 - TRL3) by technology validation in relevant environments (development levels TRL4 – TRL6) to demonstrators of prototypes (deployment levels TRL7 – TRL9). During our Workshop, to address such challenges of binding basic scientists with researchers who work at higher TRLs levels under real products we will build multidisciplinary teams. An end-user approach will allow us to study real needs and visualize particular solution and final product that we all use every day. An example of our project may be finding an environmentally friendly heating system to heat up a flat in a tenement house located in an Old Town. For that, participants of our workshop will collect an interview with a flat inhabitant including her/his preferences, financial status, etc. To support our participants in real world solutions, we will focus also on studies of real cases.

You are cordially welcome to join us!



**Tuesday morning**

**28<sup>th</sup> November 2023**

**Sessions 1 – 2**





## Single crystal growth of $\text{In}_7\text{Pd}_3$ : A case study

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Single crystalline surfaces of cubic  $\text{In}_7\text{Pd}_3$  (Pearson symbol  $cI40$ ) with various crystallographic orientations are regarded an interesting object for surface science studies with respect to their catalytic properties and would allow a comparison with the properties of the isostructural compound  $\text{Ga}_7\text{Pd}_3$  grown in an earlier project [1]. The preparation of surfaces being large enough for a couple of analytical methods needs single crystals in the size of a few  $\text{cm}^3$  which were never grown before.

Starting with the known phase diagram data (Fig. 1) [2] and some experience with Czochralski growth of single crystals in similar intermetallic systems, the crystal grower can sometimes learn a lot when doing the experiments and getting some unexpected findings. In this presentation, the originally scheduled strategy based on thermodynamic data will be discussed as well as the surprising results of a couple of experiments that failed. Finally, single crystal growth has been achieved (Fig. 2). It is the aim of this talk to present the preparation of single crystals as a scientific subject of its own rather than a production process that can be just ordered on demand.

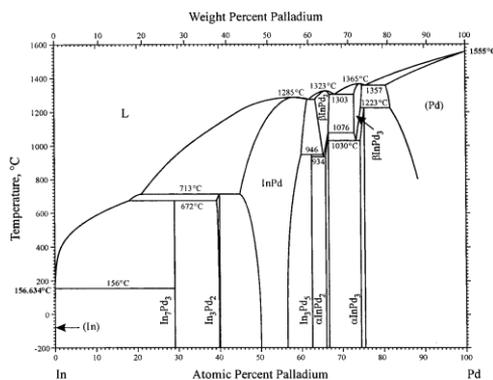


Fig. 1: In-Pd phase diagram according to [2].



Fig. 2:  $\text{In}_7\text{Pd}_3$  single crystal grown from an In-rich solution of  $\text{In}_{86}\text{Pd}_{14}$  composition. (mm grid)

### Acknowledgment

This study has been supported by palladium supply by the Université Lorraine, CNRS, IJL in common projects within the ECMetAC network.

[1] J. Schwerin, D. Müller, S. Kiese, P. Gille, J. Crystal Growth 401, 613 (2014).

[2] H. Okamoto, J. Phase Equilib. 24, 481 (2003);

H. Flandorfer, J. Alloys Compd. 336, 176 (2002).

## The structural similarity between Tsai- and Bergman-type phases

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Tsai-type quasicrystals were discovered upon isovalant substitution of Zn in Bergman-type Zn-Mg-Rare Earth system with Cd atoms [1]. It was speculated that Hume-Rothery mechanism is responsible for the stabilization of quasicrystals therefore the change between elements with the same number of valence electrons should also form a stable phase. It was revealed that the newly discovered Cd-Mg-Rare Earth quasicrystal have 10 at. % lower concentration of Mg and 5 at. % higher content of Rare Earth element. The basic structural motif is Tsai instead of the Bergman cluster.

In 2008 the structural solution of Ag-In-Yb 2/1 periodic approximant crystal of Tsai-type quasicrystal was published where pseudo-Bergman clusters were used as structure building blocks [2]. Recently, it was revealed that not only 2/1 periodic approximant structure of Tsai-type phase can be solved with Bergman clusters but the same can be done even for 1/1 approximants [3]. Additionally, Bergman phases can be solved with Tsai clusters characterized by deformations.

In this presentation the molecular orbital theory is employed to understand the similarities between Tsai-type and Bergman-type phases. By forcefully shifting atoms from their positions in the Tsai-type structure to their locations in the Bergman-like structure the modifications of the electronic structure of the subset of the ZnMgSc 1/1 periodic approximant crystal are investigated (Fig. 1). Upon performing electronic structure calculations, we conclude the structure is stabilized by hybridization of Zn4p and Sc3d orbitals. The sp band of Zn density of states is altered by the shift, increasing the occupancy of p states. The growth of the p orbitals occupancy leads to antibonding p orbitals interactions elevating the HOMO energy. HOMO/LUMO energy gap decreases. The decrease of the HOMO energy can be achieved by substituting Zn or Sc with Mg that do not contribute neither p nor d states to the highest energy orbitals.



Fig. 1. HOMO (left) and LUMO (right) for the ZnMgSc 1/1 approximant crystal

[1] J. Q. Guo, E. Abe, A. P. Tsai, *Philos. Mag. Lett.* 82, 27, (2002).

[2] M. R. Li, S. Hovmoller, J. L. Sun, X. D. Zou, K. H. Kuo, *J. Alloy. Compd.* 465, 132, (2008)

[3] I. Buganski, J. Wolny, *J. Alloy. Compd.* 939, 168823, (2023)



## The thermodynamic stability of the ThMn<sub>12</sub>-type phase in new hard magnetic (Ce,Zr,Nd)Fe<sub>10</sub>Si<sub>2</sub> alloys

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The contribution of hard magnetic materials to energy applications is essential today. On the other hand, the continuous growth of the global market of permanent magnets is subject to possible supply chain disruption. Although it is always possible to manufacture new systems with improved properties, there is a group of metastable phases that are difficult to synthesize, and the ThMn<sub>12</sub>-type phase is a good example. Several methods are used to determine the optimum compositions, with the aim of improving the structural stability and magnetic performance of new alloys.

Semi-empirical Miedema's model is used by us and the results will be discussed along with those obtained by a more sophisticated method (*ab initio* calculations). The approach is useful for mimicking the synthesis process, where different phases compete. The results of calculations will be presented together with experimental evidence for (Ce,Zr,Nd)Fe<sub>10</sub>Si<sub>2</sub> alloys consisting of a hard magnetic phase of the ThMn<sub>12</sub>-type (tetragonal structure, space group *I4/mmm*). This phase could close the performance gap between ferrite and Nd-Fe-B magnets. Further progress is mainly hindered by the low structural stability of the phase mentioned compared with other phases competing in the synthesis process, particularly those with a 2:17 stoichiometry. The results confirm the possibility of stabilizing the ThMn<sub>12</sub>-type phase even with a relatively high content of Nd, which normally tends to destabilize the desired structure.

We acknowledge the financial support of the National Science Centre Poland under the decision DEC-2021/41/B/ST5/02894 (OPUS-21).

[1] K. Koepernik, H. Eschrig, Phys. Rev. B, 59 (1999) 1743.

## Searching for new uranium-based arsenides

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Iron-based high-temperature superconductors still pose many open questions even after nearly two decades of intense research. While small energy scales of analogous actinide- and lanthanide-based materials likely prohibit existence of similarly high-temperature super-conductivity, it is certainly fruitful to investigate what happens when 4*f* and 5*f* orbitals are introduced into these structures [2]. Our previous

work, [3, 4] indicated that much can be from searching for new materials among arsenic-based systems. In this talk, I will showcase some of our recent work on the cobalt-based arsenides. We will revisit the U-Co-As ternary, in which two compounds has been reported to exist so far –  $\text{UCoAs}_2$  ( $P4/nmm$  space group) [5] and  $\text{U}_2\text{Co}_{12}\text{As}_7$  ( $P-6$  space group) [6]. By implementing flux synthesis, we were able to grow large single crystals of  $\text{UCo}_5\text{As}_3$  and  $\text{UCo}_3\text{As}_2$  compounds, which adopts own and  $\text{HoCo}_3\text{P}_2$  [7] structure types respectively.  $\text{UCo}_5\text{As}_3$  ( $P6_3/m, hP74$ ) with lattice parameters  $a = 17.7460(5) \text{ \AA}$ ,  $c = 3.8120(1) \text{ \AA}$  and  $\text{UCo}_3\text{As}_2$  ( $Pm\bar{m}n, oP38$ ) with lattice parameters  $a = 3.8623(2) \text{ \AA}$ ,  $b = 10.8416(6)$ ,  $c = 12.7265(7) \text{ \AA}$  [8]. The refined compositions agrees well with the elemental ratio established by the EDX analysis –  $\text{U}_{14.2(3)}\text{Co}_{57.3(3)}\text{As}_{28.5(3)}$  and  $\text{U}_{15.8(2)}\text{Co}_{52.2(2)}\text{As}_{32(2)}$ . The physical properties of  $\text{UCo}_5\text{As}_3$  and  $\text{UCo}_3\text{As}_2$  were studied by magnetic susceptibility measurements which revealed an antiferromagnetic ordering in both compounds below  $T_N = 25$  and 65 K, respectively. With more in-depth investigations of this and other U-Co-As ternary compounds being currently underway.

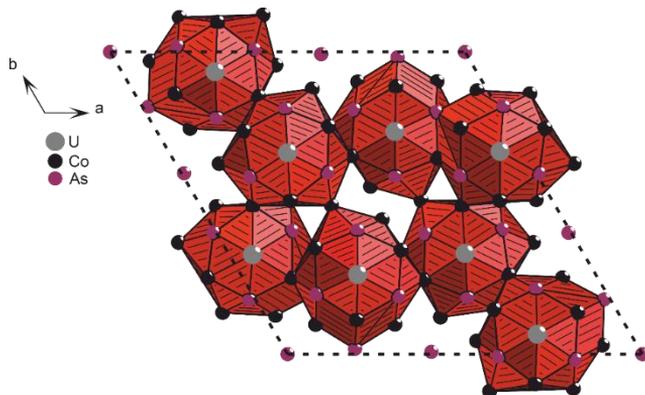


Figure 1: Crystal structure of  $\text{UCo}_5\text{As}_3$  compound, represented by stacking of U polyhedral, which are connected by common vertices and edges.

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## New Samarium Iron Arsenide $\text{SmFe}_5\text{As}_3$

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Iron-based arsenides are a promising class of materials for discovering new high  $T_c$  superconductors due to the 'pluripotency' of arsenic [1]. In particular, several iron-based superconductors with various stoichiometries have been reported, such as  $\text{LiFeAs}$  (18 K) [2],  $\text{K}_{0.6}\text{Ba}_{0.4}\text{Fe}_2\text{As}_2$  (38 K) [3],  $\text{SrFe}_2\text{As}_2$  and  $\text{BaFe}_2\text{As}_2$ , in which superconductivity is induced by pressure with  $T_c = 27$  and 29 K, respectively [4]. Surprisingly, very few rare earth-based analogs of iron arsenides have been reported so far. The search for new iron arsenides has recently led to the discovery of  $\text{EuFe}_2\text{As}_2$ , in which superconductivity can be induced by alkali metal doping or pnictogen substitution [5].

Very little work has been carried out in the ternary Sm-Fe-As system. So far, only the existence of the skutterudite  $\text{SmFe}_4\text{As}_{12}$  with ferrimagnetic transition at 29 K has been reported [6]. In this work, we revisit the Sm-Fe-As ternary. We were able to obtain the new  $\text{SmFe}_5\text{As}_3$  arsenide, which adopts the  $\text{UCr}_5\text{P}_3$  [7, 8] structure type by implementing Bi-flux method.  $\text{SmFe}_5\text{As}_3$  crystallizes in  $P21/m$  space group, with the refined lattice parameters  $a = 3.8531(4)$  Å,  $b = 7.1848(8)$  Å,  $c = 9.7103(12)$  Å, and  $\beta = 100.5(5)^\circ$ . The refined composition is in good agreement with the elemental ratio obtained from the EDX analysis. The study of physical properties of  $\text{SmFe}_5\text{As}_3$  revealed magnetic ordering below  $T_c = 84$  K, with more in-depth investigations currently underway.

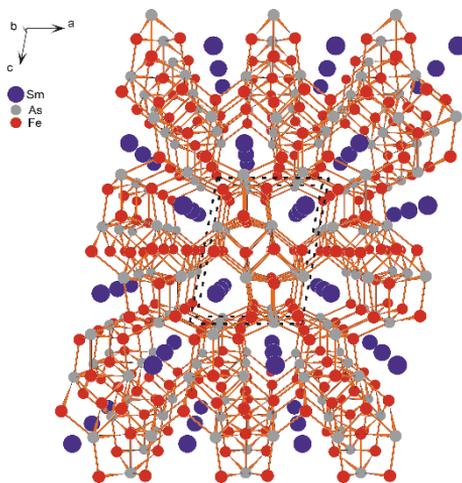


Fig. Crystal structure of  $\text{SmFe}_5\text{As}_3$  compound represented by a 3D Fe-As framework.

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## Prussian Blue Analog as a precursor for synthesizing of Ni(Fe, Co)-based nanoparticles

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Magnetic materials are nowadays broadly investigated also aiming novel green energy sources. One of the materials, which is considered as magnetically hard and destined for future applications, is NiFe-based alloy crystallizing in the L1<sub>0</sub> structure which was found firstly at meteorite. There were various attempts to obtain L1<sub>0</sub> structure, with physical and chemical methods among them, for example chemical precipitation method and reduction or rapid quenching and isothermal annealing.

NiFe-based and CoFe-based core-shell nanoparticles with carbon were prepared by use of precipitation method followed by isothermal annealing of prussian blue analogue (PBA) at 320°C. The XRD analysis of the annealed NiFe, indicated the presence of oxides and carbon. For prolonged annealing, NiFe nanoparticles with possible presence of tetrataenite (L1<sub>0</sub> structure) and Fe<sub>3</sub>O<sub>4</sub> (due to high amounts of oxygen) were reported. In the case of CoFe-based nanoparticles, mostly α-Fe crystallites are visible. One broad exothermic peak was visible on calorimetric curves for both analyzed alloys and is connected with the release of residual water and decomposition for both compounds. The Verwey transition around 113 K confirmed presence of magnetite. Crystallization of the α-Fe phase results in high saturation magnetization of above 160 emu/g for CoFe nanoparticles.

AM work was supported by the National Science Centre Poland, within the project No. 2019/35/B/ST5/01568. TM acknowledge the financial support of the National Science Centre Poland, within the projects No. 2019/35/B/ST5/01568 and 2021/41/N/ST5/01112.

## Strategies of synthesizing Prussian blue analogs of mixed composition into reduced dimensionality systems

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The idea of creating molecular magnets relies on merging different building blocks consisting of magnetic ions and organic or inorganic ligands. Such molecular magnetic nanomaterials often combine multiple attractive properties, e.g. low density, high magnetic moment per unit of volume, or sensitivity to external stimuli (temperature, pressure, etc.). Although the size reduction of a final product is usually beneficial from the application point of view, synthesizing samples into a desired shape, size, and composition is often challenging.

The results for two Prussian blue analogs' families will be presented: binary systems of  $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$  and  $\text{Fe}_3[\text{Cr}(\text{CN})_6]_2$ , and a series of compounds with mixed composition,  $\text{Ni}_3[\text{Fe}(\text{CN})_6]_x[\text{Cr}(\text{CN})_6]_{2-x}$ . We obtained the samples from the first group in the form of films and nanotubes by electrochemical deposition using different substrates [1]. For the second family, we chose sequential adsorption and ion-exchange techniques to grow two different film types, and slow precipitation to create nanoparticles.

We analyze the morphology of final products and present their structural, spectroscopic, and magnetic properties. Additionally, we fit the magnetization curves of binary systems to the mathematical model, which enables a decomposition into separate hysteresis loops (Fig. 1b). This approach helps estimate the final composition of these samples.

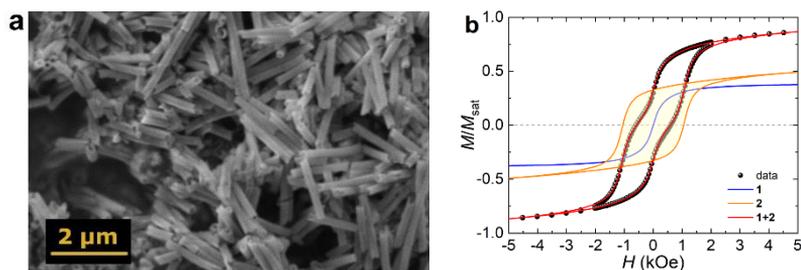


Figure 1 Double-shell nanotubes of  $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$  and  $\text{Fe}_3[\text{Cr}(\text{CN})_6]_2$ : morphology (a) and magnetic hysteresis loop decomposed into base phases (b)

**Acknowledgments:** This work was supported by the Croatian Science Foundation (project no. HrZZ IP-2020-02-9666) and National Science Centre Poland (project no. UMO-2018/31/N/ST5/03300).

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## Diverse microstructures of the magnetic high-entropy alloys

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High-entropy alloys (HEAs) represent novel metals-based materials with complicated microstructures, where at least five different chemical elements, all in majority concentrations, are mixed on a simple crystal lattice. Likewise, the materials are usually comprised of more than one phase on different microscopic levels, ranging from a few nm to 1 mm.

With the poster, I will present the microstructures of 3 different HEAs (Fig. 1), each of them presenting a special magnetic phenomena. They all possess specific two-phase nanostructure, which influences the magnetic behavior of the bulk HEA material accordingly. FeCoCrMnAl [1] is a single crystal with a two-phase structure that leads to two successive magnetic phase transitions above room temperature. This makes the material promising candidate for the application in magnetocaloric refrigeration. FeCoNiPdCu [2] is the first magnetically soft high-entropy alloy, which performs comparably to the best commercial soft magnets for static and low-frequency applications. AlCoFeNiCu [3] is a material that possess a combination of excellent magnetic softness and vanishing magnetostriction. This is beneficial for the applications that need supersilent (inaudible to a human ear) materials, like transformers, magnetocaloric coolers, and other “humming” electromagnetic machinery.

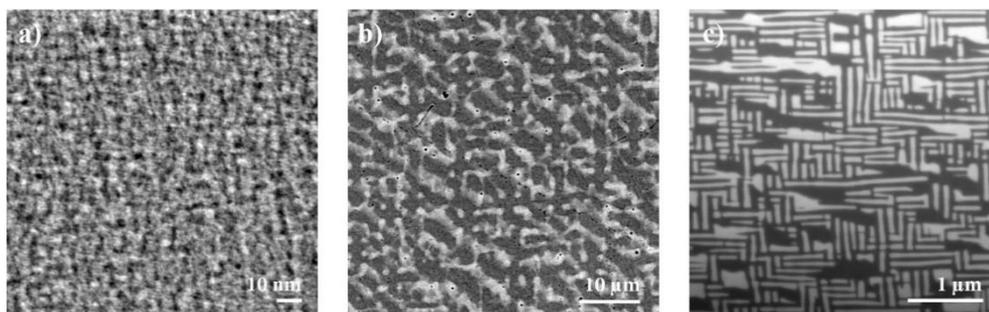


Fig. 1: Nanostructures of two-phase magnetically diverse high-entropy alloys: a) HAADF STEM image of the FeCoNiPdCu HEA material [2], b) BS SEM image of the AlCoFeNiCu HEA material [3] and c) BS FIB image of the FeCoCrMnAl HEA material [1].

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## Surface structure of $\text{In}_3\text{Ni}_2$ intermetallic compound

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Ronan McGrath<sup>1</sup>, and Hem Raj Sharma<sup>1</sup>

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Intermetallic compounds can be used as catalysts as they show better selectivity and superior long-term stability for specific catalytic reactions compared to their elemental counterparts [1].  $\text{In}_3\text{Ni}_2$  acts as catalyst for hydrogenation of carbon dioxide into methanol [2]. Understanding of surface structure and electronic properties of  $\text{In}_3\text{Ni}_2$  would help to learn and optimise the catalytical activities.

In this work  $\text{In}_3\text{Ni}_2$  intermetallic compound with (100), (001) and (2<sup>-</sup>10) orientations were investigated by X-Ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning tunneling microscopy (STM) to investigate the surface geometry in ultrahigh vacuum (UHV) at room temperature.

The surface behaviour of  $\text{In}_3\text{Ni}_2$  intermetallic has not been investigated using XPS, LEED or STM, nor have UHV studies been reported on single crystals. The only article published recently focuses on anisotropic electrical, magnetic, and thermal properties [3].

All high symmetry surfaces (100), (001) and (2<sup>-</sup>10) prepared by sputtering (Ar<sup>+</sup> for 30 minutes, drain current 5-6  $\mu\text{A}$ ) and annealing at 310-560 °C were studied. We found that surface ordering and high-quality LEED patterns starts at annealing temperature of 340 °C. LEED patterns for two surfaces (100) and (2<sup>-</sup>10) reveal bulk truncated surface, (1x1) structure. However, the (001) surface has two different types of surface reconstructions C-(3x  $\sqrt{3}$ ) and c-(2 $\sqrt{3}$  x 4) rectangular with three different domains.

Atomic resolution is obtained in STM images, which can be explained using the model atomic structure. There is (1x1) surface structure confirmed by STM for  $\text{In}_3\text{Ni}_2(100)$  and  $\text{In}_3\text{Ni}_2(2-10)$ . Furthermore, the (001) surface shows a c-(2 $\sqrt{3}$  x 4) rectangular superstructure with three domains and (3x  $\sqrt{3}$ ) reconstruction that formed from deposit H<sub>2</sub>-deposition, which is confirmed by both LEED and STM.

After evaluation of XPS data measured from  $\text{In}_3\text{Ni}_2$  with three different orientations, we found that In is preferentially sputtered leaving more Ni on the On- the other hand, annealing the surface at 310 °C to 560 °C promotes segregation of In onto the surface.

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**Tuesday afternoon**

**28<sup>th</sup> November 2023**

**Sessions 3 – 4**





## Topological semimetals in strongly correlated systems

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Gapless electronic topology driven by strong correlations is an emerging field of great interest, with heavy fermion compounds at its forefront. I will introduce the first such materials class, Weyl-Kondo semimetals [1-3], and report on the giant signatures of topology observed in  $\text{Ce}_3\text{Bi}_4\text{Pd}_3$  [1,3] and the genuine topology control that can be achieved by magnetic field tuning [4,5]. I will also discuss design strategies for further correlation-driven topological phases, and discuss several realizations [6,7].

This work was supported by the Austrian Science Fund (FWF-I4047, I5868-FOR5249-QUAST, SFB F 86, Q-M&S), the European Union's Horizon 2020 Research and Innovation Programme (824109, EMP), and the European Research Council (ERC Advanced Grant 101055088, CorMeTop).

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## Kondo effect in $\text{Ce}_x\text{LaLuScY}$ ( $x = 0.05\text{--}1.0$ ) high-entropy alloys

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The original definition proposed by Yeh et al. in 2004 describes high-entropy alloys (HEAs) as alloys with multiple principal elements in equimolar or near-equimolar ratios, whose high entropy of mixing enhances stabilization of single-phase random solid solution on simple crystal lattices. Almost two decades later, research and understanding of physical phenomena appearing in HEAs until today remains relatively scarce.

Our motivation was to try and expand the area of HEAs to correlated-electron systems, where we designed and synthesized a series of hexagonal rare earths based HEAs with nominal formula  $\text{Ce}_x\text{LaLuScY}$  ( $x = 0.05, 0.1, 0.2, 0.5$  and  $1.0$ ), with Ce being the only element that possesses a magnetic moment, while the rest four elements are nonmagnetic.

This presentation will mainly cover the measurements and analysis of electrical resistivity, magnetic susceptibility and specific heat, which revealed that  $\text{Ce}_x\text{LaLuScY}$  HEAs show the Kondo effect. While alloys can be classified as dense Kondo systems, the results support the presence of a single-impurity Kondo effect across the entire range of Ce concentrations.

In addition, main results will be preceded with short insights on materials' characterization, i.e., motivation for synthesis and determination of crystal structure, lattice parameters and chemical composition for all samples.

*Acknowledgments:* This research has been financially supported by the Slovenian Research and Innovation Agency (research core funding No. P1-0125).

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## Anisotropic thermal conductivity of hydrogen fuel cell catalyst films

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Goal of our research is development of a proton exchange membrane (PEM) with increased lateral thermal conductivity to improve hydrogen fuel cell efficiency and longevity. PEMs in polymer electrolyte fuel cells belong to a class of materials known as ionomers. These materials exhibit anisotropic thermal conductivity which depends highly on chemical composition, degree of hydration, size of water domains surrounded by polymer chains whose geometry is influenced by the stress and strain induced in the membrane during operation by local overheating.

Frequency domain measurement techniques ( $3\omega$  method [1]) with arbitrary sensor geometries enable measurement of the general thermal conductivity tensor. Finite element simulations are used to model arbitrary heater geometries to interpret experimental results.

Thermal conductivity of the sensor substrate was measured and results are consistent with literature. Thin ionomer film was applied on top of the sensor and the ionomer + sensor substrate system thermal conductivity was measured in the operating temperature range of the hydrogen fuel cell under vacuum.

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## Effect of Al-Cu-Fe Quasicrystal particles on the reinforcement of a polymer-matrix composite: from mechanical to surface properties

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Gaël Pierson<sup>e</sup>, Richard Kouitat<sup>e</sup>, Jean-Marie Dubois<sup>a, b</sup>, Sašo Šturm<sup>a, b, f</sup>

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Quasicrystals (QCs) combine high hardness with low adhesion energy, making them ideal for applications that require non-stick properties [1]. Our expectation was that novel composites based on quasicrystals would maintain their functionality and resist fatigue failure and wear, even when subjected to long-term use under normal or extreme conditions.

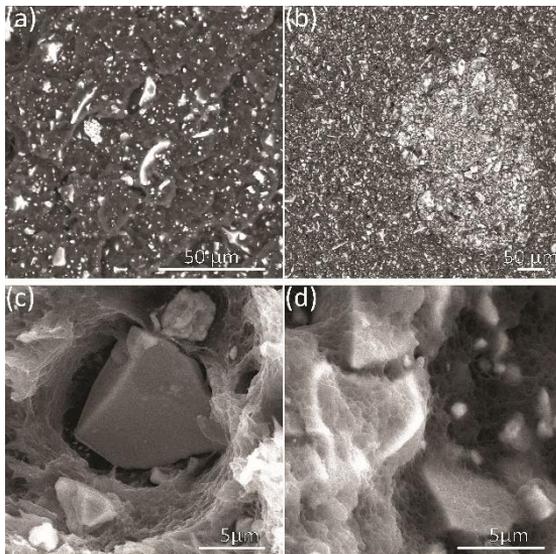


Fig. 1: SEM/BSE images of the fracture surface after tensile testing for the composite material with different volumes of filling particles: (a) PPA with 20 vol.% of QC and (b) PPA with 35 vol.% of QC, (c) characteristic higher-magnification micrograph of the PPA with 5 vol.% of QC and (d) high-magnification micrograph of the PPA with 20 vol.% of QC.

We explored the feasibility of creating a unique combination of the best attributes of Polyphthalamide (PPA), a technical polymer, and a quasicrystalline material to enhance such a composite's surface and mechanical properties. Scanning electron microscopy (SEM) was used to specify the microstructure of the composite materials with different fillings of  $\text{Al}_{59}\text{Cu}_{25}\text{Fe}_{13}\text{B}_3$  (at.%) QC into the polymer matrix (Fig. 1). The surface energy deduced from the contact angle measurements was found between 36 – 39  $\text{mJ/m}^2$  for the composites, which shows a good match to both the naked polymer (39  $\text{mJ/m}^2$ ) and the QC equipped with his native oxide layer in the air (average around 37  $\text{mJ/m}^2$ ). A clear minimum of the surface energy was found for the composite material with 20 vol.% of QC filling, in association with a net drop of the polar component of the surface



energy. The investigated materials exhibit a percolation threshold at about 13 vol.% QC contents, reflected in the observed behaviour of the impact strength and friction coefficient. This research shows that by combining the favourable properties of QCs and polymers, the studied materials have potential value for technological applications.

#### Acknowledgement

This work was performed within the frame of the International Research Project (IRP) PACS2. The research was financially supported by the Slovenian Research Agency (P2-0084), CNRS and Université de Lorraine, France, and the European Union Horizon 2020 research and innovation programme under grant agreement No. 823717 – ESTEEM3.

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## Stability and electronic properties of two-dimensional oxide quasicrystal approximants

Weiliang Ma<sup>1</sup>, Thiago Trevizam Dorini<sup>1</sup>, Florian Brix<sup>1,2</sup>, Émilie Gaudry<sup>1,2</sup>

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Ultra-thin films of oxide quasicrystals supported on metallic surfaces represent promising materials from both the basic science and technological application. Due to the absence of periodic boundary conditions, oxide quasicrystals adopt various forms on the substrate surfaces. Nevertheless, only a few oxide quasicrystalline approximants (OQAs) such as the sigma phase, giant approximant, and hexagonal approximant<sup>[1]</sup> have been observed in experiments, raising questions about the stability of quasiperiodic order in these systems. Several key factors governing the formation of new oxide structures have been reported, including the effects of size mismatch and the dipole between the two separate systems. We demonstrate that the density of transition metal elements in proximity to the support substrate can also play a crucial role. In this study, we have developed a new modeling method to generate the approximants flexibly and automatically. To investigate the stability of OQAs, we have generated 30 different approximants belonging to three different alkaline-earth metals group within the Niizeki-Gähler tiling. The structural, thermodynamic, electronic, and work functions of two-dimensional OQAs supported on metallic substrates have been systematically investigated to uncover the structure-stability-property relationships. This study offers well-founded insights into the factors of electronic effects on the stability of this system, providing a guideline for identifying suitable candidates for future experiments.

[1] Merchan, C. Ruano, et al. Two-dimensional square and hexagonal oxide quasicrystal approximants in SrTiO<sub>3</sub> films grown on Pt (111)/Al<sub>2</sub>O<sub>3</sub> (0001). *Physical Chemistry Chemical Physics* 24.12 (2022): 7253-7263.



## Transformation of two-dimensional quasicrystalline approximants into partially filled honeycomb lattices in reduced SrTiO<sub>3</sub> thin films supported on Pt(111)/Al<sub>2</sub>O<sub>3</sub>(0001)

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Two-dimensional oxide quasicrystals have been observed for Ba-Ti-O [1] and Sr-Ti-O [2] ultra-thin films supported on hexagonally closed-packed metal substrates. In a recent work, a new square approximant with a giant unit cell as well as an hexagonal phase have been reported using an all-thin-film approach where the metal single crystal is replaced by a 10 nm thick Pt-(111) buffer layer grown on an Al<sub>2</sub>O<sub>3</sub>(0001) substrate by molecular beam epitaxy, whereas the oxide film is grown by pulsed laser deposition [3]. Here, we report the transformation of these quasicrystalline approximants into Sr decorated Ti<sub>2</sub>O<sub>3</sub> honeycomb lattices upon annealing in ultra-high vacuum, a reduction process that shifts the composition of these ultra-thin oxide films away from the initial perovskite composition.

A 'labyrinthic' phase as well as a partially ordered  $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$  phase will be reported. These results are consistent with a recent proposal based on density functional theory (DFT) calculations that quasicrystals/approximants can be transformed into Sr decorated Ti<sub>2</sub>O<sub>3</sub> honeycomb lattices through low-energy defects identified as Stone–Wales transformations, typical of hexagonal 2D materials [4]. We also present some preliminary studies on the SrRuO<sub>3</sub>/Pt(111)/Al<sub>2</sub>O<sub>3</sub>(0001) oxide films which have not been explored so far using a similar approach.

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## Epitaxial CoCrFeNi films for surface investigations

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High-entropy alloys (HEAs) are discussed for applications in the fields of corrosion and wear protection as well as electrocatalysts. Although the surface properties of HEAs play a central role in these applications, they are still largely unexplored, which is to a certain extent caused by a lack of sample availability. In this presentation recent progress is reported on the growth and subsequent characterization of epitaxial CoCrFeNi films [1]. The films were grown by DC magnetron sputtering from spark-plasma sintered targets [1] using single-crystalline oxide substrates. Characterization was performed by a variety of different techniques including X-ray diffraction (XRD), scanning electron and transmission electron microscopy (SEM, TEM), energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), angle-resolved photoelectron spectroscopy (ARPES), low-energy electron diffraction (LEED) and, more recently, by scanning tunnelling microscopy (STM).

As an example, figure 1 shows an STM image of CoCrFeNi(100). The surface shows steps with a minimum height of 1.8 Å, which is half the lattice constant of the alloy, as well as steps with heights corresponding to integer multiples thereof. Some examples are marked in figure 1. Screw dislocations (SDs, marked by green dots) can be identified by the appearance of steps with a height of 1.8 Å inside a terrace. Most striking is the observation of a patch work like nanostructure. It is recognizable by virtue of the vertical and horizontal dark lines in figure 1. They are due to depressions in the apparent height of about 60 pm and part the surface in patches of approx. 3 nm by 3 nm in size. The origin of this interesting feature is currently not understood. The potential of epitaxial HEA films for surface science and catalysis studies is discussed.

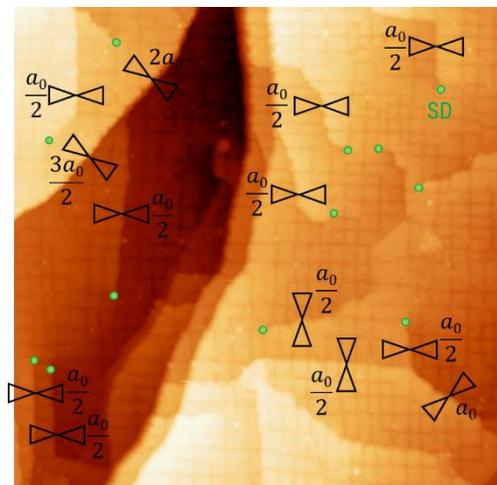


Figure 1: STM image of CoCrFeNi(100) (size 90 nm × 900 nm, U = -1.0 V, I = 0.08 nA, z-scale: 0 - 2.375 nm).

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**Wednesday morning**

**29<sup>th</sup> November 2023**

**Sessions 5 – 6**





## Rare-Earth High Entropy Alloy Thin Films

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High entropy alloys (HEA) refer to metallic random solid solution made of at least five elements each of which in an equi- or near-equiatomic concentration. Initially under scrutiny for their exceptional mechanical properties, the surface properties of the materials have recently been the focus of interest including their oxidation, corrosion and wear resistance, and their catalytic activity. With an immense compositional space, it is certain that many compositions will continue to emerge each with novel bulk or/and surface properties. To this end, it is crucial to understand the chemical and structure evolutions of HEA under different environments. Our attention has been attracted to the fundamental study of HEA surface under ultra-high vacuum conditions aiming to answer key questions related to surface phenomena at the atomic level [1]. To continue this approach, the growth of HEA in the form of thin films offers a convenient solution [2] to face the difficulty encountered with the availability of centimetre-size HEA single crystals, often considered as model systems.

Here, we report the successful epitaxial growth of a quinary HEA thin film using molecular beam epitaxy (MBE). A 95 nm thick DyGdHoLuTb has been grown on a 30 nm Nb buffer layer deposited on sapphire. The layer thicknesses are determined by reflectivity measurements while x-ray diffraction measurements coupled with cross-sectional transmission electron microscopy analysis reveal the growth of a random solid solution of hexagonal close packed structure. With sharp interfaces between the deposited layers, energy dispersive x-ray spectroscopy measurements indicate a homogeneous chemical distribution among the elements. Once inserted under ultra-high vacuum conditions, the thin film surface has been prepared by Ar<sup>+</sup> sputtering and annealing cycles to various temperatures. The DyGdHoLuTb(0001) surface is unreconstructed and well-ordered as revealed by a sharp six-fold low energy electron diffraction pattern. Scanning tunnelling microscopy images show a step and terrace morphology with a single step height equal to  $c/2$ . *Ex situ* magnetic measurements carried out on the thin film replicate the main characteristic of the magnetic field–temperature ( $H$ ,  $T$ ) phase diagram reported on polycrystalline samples apart from a low temperature spin-glass state [3].

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## C<sub>60</sub> adsorption on the (100) surface of Au-Si-Ho Tsai-type approximant

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Au-Si-Ho Tsai-type 1/1 approximants structures are built from a specific cluster type where the central disordered tetrahedron can be partially or totally replaced by a Ho atom leading to alteration of magnetic and thermoelectric properties[1]. Unlike for the bulk, the surface atomic structure and the reactivity of Au-Si-Ho systems remain unexplored. To this end, we report the characterization of the (100) surface of the Au<sub>4.85</sub>Si<sub>1.324</sub>Ho<sub>0.04</sub> Tsai-type 1/1 approximant using both experimental techniques and Density Functional Theory (DFT)-based methods. Low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) show a (2x1) surface reconstruction. The patterns present on the surface are comparable to the patterns present on one of the bulk planes for which DFT calculations were performed. The reactivity of this surface was studied by C<sub>60</sub> adsorption. Adsorption of C<sub>60</sub> on Au-Si-Ho is disordered at room temperature but ordered at 669 K. In the submonolayer regime with the sample held at 669 K, different superstructures are observed ((1x1), ( $\sqrt{2}/2 \times \sqrt{2}/2$ )R45°) depending on the fullerenes coverage. Upon completion of the first monolayer of C<sub>60</sub>, the thin film of ( $\sqrt{2}/2 \times \sqrt{2}/2$ )R45° superstructure can be regarded as a (100) surface of the face centered cubic structure of C<sub>60</sub>. The highest symmetry matching between the C<sub>60</sub> molecule and the surface is obtained when a pentagonal face of the C<sub>60</sub> molecule is facing the surface at specific surface atomic sites. We will present the potential 5-fold adsorption sites identified on the Au-Si-Ho(100) surface.

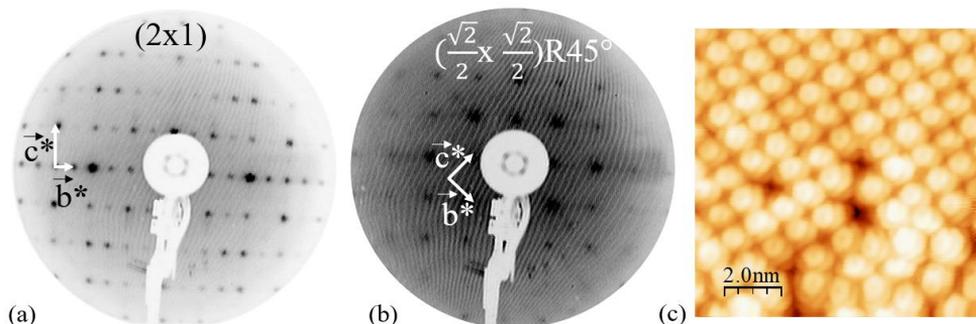


Figure 1 : LEED pattern recorded at 22 eV for a clean surface (a) and after dosing 1 monolayer of C<sub>60</sub> (b). (c) STM image recorded at -1.80 V after dosing 0.8 monolayer of C<sub>60</sub>.

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## Structural, Ordering, and Magnetic Properties of PtNi Nanoalloys Explored by Density Functional Theory and Stability Descriptors

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Monometallic platinum and nickel nanoparticles and platinum–nickel nanoalloys are examined in the range 13–976 atoms from density functional theory calculations (a few examples are given in Fig 1). A large set of competitive symmetries and morphologies are considered including the usual Mackay icosahedral, Marks decahedral, and truncated octahedral forms. A comparative analysis of relative stability order is addressed on the basis of four stability descriptors all predicted at the *ab initio* level from spin-polarized calculations including van der Waals interactions. For platinum nanoparticles, they unanimously conclude on the preference of truncated octahedral morphology in the range of 147–201 atoms. For nickel and platinum–nickel nanoclusters, three descriptors (cohesion energy, nanoparticle

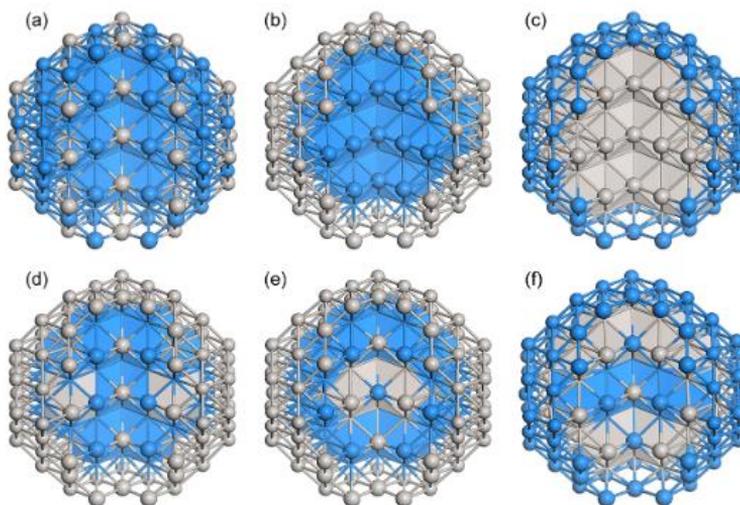


Figure 1: Families of chemical ordering in PtNi nanoalloys in the case of 201-atom nanoclusters: (a) crystalline Pt<sub>57</sub>Ni<sub>144</sub> (1 example) versus (b–f) noncrystalline nanoalloys (five examples); (b, c) core–shell Pt<sub>122</sub>Ni<sub>79</sub> and Pt<sub>79</sub>Ni<sub>122</sub> (Pt-skin and Ni-skin, respectively), (d) skin–heart Pt<sub>141</sub>Ni<sub>60</sub> (1 example); (e, f) multishell Pt<sub>140</sub>Ni<sub>61</sub> and Pt<sub>61</sub>Ni<sub>140</sub> (Pt-skin and Ni-skin, respectively). Pt atoms are depicted in gray and Ni in blue. To show the chemical ordering inside the clusters, a slice has been systematically canceled laterally. Surface and interior atoms (visible after being stripped) are drawn with balls while core atoms with solid representation.



surface energy, and vibrational band center) also support such octahedral symmetry (with a skin–heart chemical ordering for nanoalloys), whereas the excess energy rather favors the icosahedral morphology (with multishell and core–shell arrangement). Such discrepancies feed the debate related to the impact of normalization on the predictive power of these descriptors and recall the high importance of validating theoretical models from a quantitative standpoint. This work invites the experimentalists to synthesize, characterize, and measure surface energetics of PtNi nanolloys in highly controlled operating conditions.



## Characterization of Co-Fe-Ni-Cu-based multi-principal element alloys

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Multi-principal element alloys containing Co, Fe, and Ni belong to magnetically soft materials. Mixing these magnetic elements with non-magnetic counterparts can result in a combination of properties that do not typically occur in conventional alloys. In this study, the effect of copper content on the microstructure and properties of CoFeNiCu-based multi-principal element alloys was investigated. Five alloys, denoted as CoFeNiCu<sub>x</sub> ( $x = 0, 0.5, 1.0, 1.5, \text{ and } 2.0$ ), were prepared using the arc-melting technique. The CoFeNi alloy consisted of a single FCC phase, designated as FCC – 1. As copper is added to the alloy and its amount increases relative to the other elements, a Cu-rich secondary FCC phase, referred to as FCC – 2, gradually forms. In this contribution, the microstructure characterization of the prepared alloys will be presented, along with some preliminary results on their mechanical properties.

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## Interplay of electronic structure and electrochemical efficiency in cathode materials for Li- and Na-ion batteries

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It is well-known that crystalline materials exhibiting specific properties may convert different forms of energy due to thermoelectric, electrochemical or magnetocaloric phenomena. The efficiency of such effects is partly related to specific electronic properties that are responsible for transport, magnetic or electrochemical behaviours. Although Li-ion battery materials are still considered to be the most promising energy converter due to their excellent electrochemical parameters, many efforts have been recently undertaken to find alternative cathode materials conducting for instance Na ions. Here, the results of electronic structure calculations of operating and potential materials for Li- and Na-ion battery systems, based essentially on  $AMO_2$  compounds ( $A=Li, Na$  and  $M= Mn, Fe, Co, Ni$ ) and their alloys, are discussed. Noteworthy, theoretical results obtained using DFT techniques (KKR and KKR-CPA) allowed to interpret the step-like (undesirable) vs. continuous-like (desirable) character of discharge curve in terms of correlations between electronic structure and electrochemical properties in known materials [1]. In next step, *ab initio* computations of a novel variant of cathodes  $Li_xCo_{1-y-z}Ni_yMn_zO_2$  [2], accounting for chemical disorder (Li vacancy and Co/Ni/Mn alloying), resulted in specific evolution of density of states in investigated range of Li contents and alloy compositions. It was predicted that electronic structure might exhibit semiconducting-like, half-metallic-like or metallic-like properties depending on Li concentration as well as relative stoichiometry of transition metal elements (Co, Ni and Mn). Moreover, the spin-polarised KKR-CPA computations resulted in magnetic moment onset, which markedly affect the overall DOS shape near  $E_F$  [3]. Furthermore, the similar calculations have been successfully employed to study particular behaviours in high-entropy oxides  $Na_xTi_{1/6}Mn_{1/6}Fe_{1/6}Co_{1/6}Ni_{1/6}Cu_{1/6}O_2$  for cathodes with high configuration entropy. Favourable correlations between the variation of Fermi energy along density of states with Na content in highly disordered ion-battery materials were found [4, 5].

In summary, specific electronic structure features appearing in ion-battery (step-like vs. continuous-like character of discharge curve, effect of high configuration entropy, effect of magnetism) evidently determine their electrochemical performance.

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## Compositionally complex alloys: some insight from photoemission and magnetism

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Several years ago, we noted a lack of experimental results for electronic structure of compositionally complex alloys (CCA) which is detrimental both to their understanding and potential applications [1,2]. More recently we have shown how photoemission spectroscopy results can simply explain physical properties of CCAs showing both a split- and common-band shape of their electronic density of states (DOS) [3,4,5]. Here, in addition to showing the correlation between the photoemission spectra and the magnetic and some other properties of selected alloys with both shapes of DOS we also show the correlation between the calculated DOS and that depicted by corresponding photoemission spectra, “experimental” DOS. Despite some similarity between the shapes of theoretical and corresponding “experimental” DOS there is significant quantitative difference between two DOS in all studied CCAs. The complexity of local atomic configurations in CCAs may possibly explain this discrepancy [6].

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## Scrutinizing the phonon Kondo effect in intermetallic clathrates

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Intermetallic clathrates are under active investigation, both for their potential in thermoelectric applications and for fundamental interest. A key characteristic of these materials is the special guest-host crystal structure “G<sub>8</sub>H<sub>46</sub>”, where the rattling motion of guest (G) atoms in oversized cages of an essentially covalently bonded host (H) framework is directly linked to unusual lattice dynamics. It is now well documented that intermetallic clathrates exhibit energetically low-lying optical phonon modes, so called Einstein modes, which strongly interact with the acoustic modes [1,2,3]. Recently, a phonon-Kondo effect was suggested to explain striking deviations between lattice dynamics predictions [4] and experimental observations for various thermal transport and thermodynamics quantities. It was proposed that a Kondo-like interaction between the lowest-energy Einstein mode, the localized entity (the “spin”), and the acoustic mode which represents the extended wave (“conduction electron”), is responsible for this deviation [5].

In our recent inelastic neutron scattering investigation we shed light on this picture, by mapping the temperature dependence of the low-energy phonon dispersion of the type-I clathrate Ba<sub>8</sub>Cu<sub>4.8</sub>Ge<sub>40.2</sub>Ga in the vicinity of the strongest optic-acoustic mode interaction. We discover a clear temperature dependence above the characteristic phonon Kondo temperature of about 40 K for this compound. I will discuss the form of this dependence and how it changes as function of the wave vector  $k$ , as well as the implications of these results.

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## Two parallel conducting channels in compositionally complex amorphous alloys of early and late transition metals

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We present a comprehensive study on the transport properties of compositionally complex amorphous alloys of early (TE) and late transition metals (TL). Our research focused on metallic glass ribbons from three alloy systems:  $(\text{TiZrNbNi})_{1-x}\text{Cu}_x$ ,  $(\text{TiZrNbCu})_{1-x}\text{Ni}_x$ , and  $(\text{TiZrNbCu})_{1-x}\text{Co}_x$ , with a broad composition range, along with three alloy variants with fixed TL (Cu, Ni) content:  $\text{Ti}_{0.30}\text{Zr}_{0.15}\text{Nb}_{0.15}\text{Ni}_{0.20}\text{Cu}_{0.20}$ ,  $\text{Ti}_{0.15}\text{Zr}_{0.30}\text{Nb}_{0.15}\text{Ni}_{0.20}\text{Cu}_{0.20}$ , and  $\text{Ti}_{0.15}\text{Zr}_{0.15}\text{Nb}_{0.30}\text{Ni}_{0.20}\text{Cu}_{0.20}$  [1, 2]. We also conducted measurements on an amorphous thin film of TiZrNbCuNi, deposited on a SrLaAlO<sub>4</sub> substrate using pulsed laser deposition (PLD).

All the measured samples showed high resistivities ( $>140 \mu\Omega \text{ cm}$ ) and a small negative temperature coefficient of resistance (TCR), in agreement with binary TE-TL alloys [3]. For the temperature variation of resistivity, we propose a novel model featuring two parallel conducting channels: a metal-like channel and a variable range hopping (VRH) like channel with a  $p=1/2$  exponent. We found that this model more accurately describes the temperature variation of resistivity than does the existing model, which attributes the negative TCR to the temperature variation of the weak localization contribution to resistivity [3].

We propose that these two parallel conducting channels are the result of the formation of regions of delocalized and localized states. The delocalised states form an infinite cluster that contributes the metal-like channel. Its temperature dependence at higher temperatures ( $\gtrsim 20\text{K}$ ) is dominated by elastic scattering on the disordered lattice, resulting in a constant resistivity value, and at lower temperatures ( $\lesssim 20\text{K}$ ) by weak localization and/or enhanced electron-electron interactions.

The infinite cluster of delocalised states also contains "dead ends" that do not directly contribute to the metallic conductance. Hopping between these dead ends and finite clusters within the sample creates conducting channels parallel to the infinite cluster. It is these channels that contribute the VRH-like component of the resistivity. We draw parallels between this VRH-like channel and the VRH observed in granular metals [4].

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## Magnetism in a nanostructured single-crystalline $\text{Al}_{28}\text{Co}_{20}\text{Cr}_{11}\text{Fe}_{15}\text{Ni}_{26}$ high-entropy alloy

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Most high-entropy alloys (HEAs) that are actively researched today are multiphase systems – sometimes as a side product of the synthesis procedure but even more often intentionally as a means to optimize their properties. The multiphase nature of these HEAs even further complicates the analysis and interpretation of the magnetism in these materials, which are already non-trivial due to the many atomic species and many types of magnetic interactions (e.g. Fe-Co, Co-Co, etc.) present in them. A recent publication [1] has analysed the complex magnetism in the  $\text{AlCo}_{0.5}\text{Cr}_{0.5}\text{FeNi}$  HEA, which exhibits hierarchical phase separation, via electron microscopy, APT and magnetic imaging.

This contribution (based on Ref. [2]) aims to complement the information about the magnetism in the Al-Co-Cr-Fe-Ni multiphase alloys via bulk magnetic studies on a broad temperature range from 2 K to 400 K. Our sample with composition  $\text{Al}_{28}\text{Co}_{20}\text{Cr}_{11}\text{Fe}_{15}\text{Ni}_{26}$  and grains of cca 1 mm<sup>3</sup> volume was synthesized with the Czochralski method [3]. Instead of a hierarchical phase separation, a nanocomposite consisting of a B2 matrix was obtained with the A2 phase taking the form of spherical nanoparticles of dimension  $64 \pm 10$  nm. The matrix does not contain anti-ferromagnetic Cr and is thus a disordered ferromagnet, which in the bulk magnetic measurements shows up as a ferromagnetic transition at cca 390 K. The spherical A2 nanoparticles are Co-Cr-Fe, likely with the outer shell enriched in Co and Fe. The mixed and frustrated ferro- and antiferromagnetic interactions in the cores of the A2 result in an asperomagnetic magnetic state. This asperomagnetic state can be seen as a non-ergodic regime below 15 K visible in the form of zfc-fc splitting in the temperature-dependent magnetization, in the frequency dependence of the AC susceptibility and through thermoremanent magnetization measurement. No collective magnetic state of the B2 matrix and A2 nanoparticles with significant interactions between them forms, so the magnetism is a simple sum of their independent magnetisms.



Figure: Nanocomposite morphology (A2 nanoparticles in a B2 matrix) of  $\text{Al}_{28}\text{Co}_{20}\text{Cr}_{11}\text{Fe}_{15}\text{Ni}_{26}$  as visible in HAADF-STEM.

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**Wednesday afternoon**

**29<sup>th</sup> November 2023**

**Sessions 7 – 8**





## Temperature-dependent frequency in the quantum oscillations of the $\text{Bi}_{1.1}\text{Sb}_{0.9}\text{Te}_2\text{S}$ topological insulator

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We introduce a Sn-doped  $\text{Bi}_{1.1}\text{Sb}_{0.9}\text{Te}_2\text{S}$  topological insulator, which stands out as a rare instance displaying temperature-dependent frequency in quantum oscillation. This material exhibits pronounced oscillations that can be attributed to its surface states. Notably, the oscillation frequency exhibits significant temperature dependence, with a decrease in value of approximately 10% within a temperature range spanning from 2 K to 40 K. The magnitude of this reduction surpasses what would be anticipated based solely on topological and Sommerfeld corrections for a Dirac band, accounting for only a quarter of the overall observed change. This suggests a noteworthy contribution from the temperature-driven dynamics of the chemical potential of the Sn-created impurity band. Various measurements, including electrical resistivity, quantum oscillations, Seebeck, ARPES, and Hall measurements, consistently place the Fermi energy within the energy gap and approximately 100 meV above the Dirac point.



## Electronic structure of (Co,Ni)<sub>1/3</sub>NbS<sub>2</sub> studied by angle-resolved photoelectron spectroscopy

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Latest discoveries of novel magnetic phases and anomalous magneto-transport behaviors in transition metal intercalated NbS<sub>2</sub> [1] have been attracting considerable attention to the systems. The host 2H-NbS<sub>2</sub> is a superconductor below 6 K [2]. Intercalation of Co/Ni atoms suppresses the superconductivity, and introduces antiferromagnetic ordering in both Co<sub>1/3</sub>NbS<sub>2</sub> and Ni<sub>1/3</sub>NbS<sub>2</sub> at T<sub>N</sub>~26 and 95 K, respectively [3]. The electronic and magnetic properties of these systems had been discussed in the frame-work of the rigid-band-model, though the recent angle-resolved photoelectron spectroscopy (ARPES) on Cr<sub>1/3</sub>NbS<sub>2</sub> casted a doubt on the validity of the model [4]. In order to study the impact of Co/Ni intercalation on the electronic structure of the host 2H-NbS<sub>2</sub>, we performed ARPES on Co<sub>1/3</sub>NbS<sub>2</sub> and Ni<sub>1/3</sub>NbS<sub>2</sub>. Our experiments revealed clear band dispersions and Fermi surfaces in both Co<sub>1/3</sub>NbS<sub>2</sub> and Ni<sub>1/3</sub>NbS<sub>2</sub>. The band dispersions exhibited similar feature to those of 2H-NbS<sub>2</sub>, with an energy shift due to charge transfer from intercalated Co/Ni to NbS<sub>2</sub> layers. Additionally, a clear non-rigid band like modification was observed in the vicinity of the Fermi level, manifesting as a shallow electron pocket originating from the intercalated atoms. [3]. The character of the bands was further investigated with the help of theoretical calculations. Our study underscores the significance of strong electron correlations in elucidating the essential features of Co<sub>1/3</sub>NbS<sub>2</sub> and Ni<sub>1/3</sub>NbS<sub>2</sub>.

This work has been partly supported by the Croatian Science Foundation under the project numbers IP 2020-02-9666 and UIP 2019-04-2154, and by the project Cryogenic Centre at the Institute of Physics – KaCIF co-financed by the Croatian Government and the European Union through the European Regional Development Fund-Competitiveness and Cohesion Operational Programme (Grant No. KK.01.1.1.02.0012).

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## Quantum phase transition in Ce<sub>3</sub>Al studied by muon spin rotation experiment

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We have experimentally studied the magnetic field-driven quantum phase transition (QPT) in the monocrystalline Ce<sub>3</sub>Al intermetallic compound. The QPT is of the spin-flip type, with a transition from antiferromagnetic (AFM) ordered to the disordered quantum paramagnetic spin state. Static aspects were investigated by experiments in a magnetic field up to 9 T and at temperatures down to 350 mK. It was shown that the external magnetic field in the (*a*,*b*) easy plane drives the AFM transition continuously towards absolute zero, while along the perpendicular *c*-direction, the QCP does not occur due to large magnetocrystalline anisotropy [1]. The Ce moments are not static even at zero temperature but exhibit quantum fluctuations in their direction due to the Heisenberg uncertainty principle. To investigate these dynamical aspects, we performed muon spin rotation ( $\mu$ SR) experiments in the temperature range between 1.5 K and 80 mK [2]. The measurements show that the fluctuations exhibit the largest amplitude at the QCP, manifesting as a maximum of the muon transverse relaxation rate  $\lambda_1$  at the critical field  $B_C$ . The quantum nature of fluctuations is reflected in the temperature independence of the average local magnetic field (Fig. 1) and the muon transverse relaxation rate (Fig. 2). The theoretical model of the relaxation rate showed that quantum fluctuations are fast in comparison with the muon Larmor frequency,  $\tau_0 < 10^{-10}$  s.

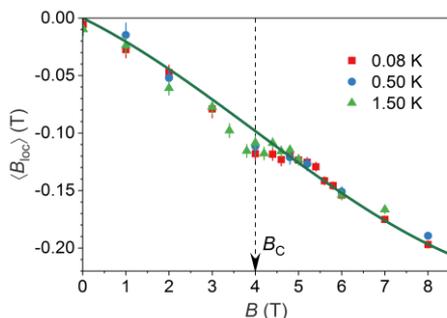


Figure 1: Average local magnetic field  $\langle B_{loc} \rangle$  at the muon stop site vs.  $B$ .

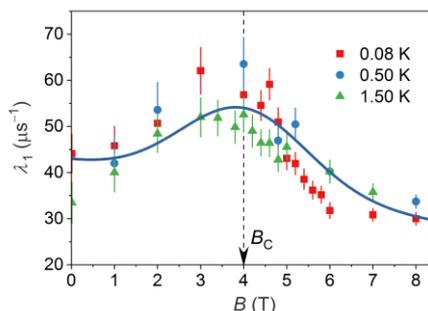


Figure 2: Muon transverse relaxation rate  $\lambda_1$  vs. external magnetic field  $B$ .

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## Electronic structure and thermoelectric performance of $\text{Ni}_x\text{Au}_{1-x}$ metallic binary alloy

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While historically the thermoelectric effect has been first discovered in metals, for many years scientific interest was focused on the semiconductors as their performance was superior to metallic alloys.

Recently,  $\text{Ni}_x\text{Au}_{1-x}$  binary metallic alloy was discovered to possess extraordinary thermoelectric performance, with power factor up to  $34 \text{ mWm}^{-1}\text{K}^{-2}$  that doubles current known values for any bulk material above room temperature [1]. The measured  $zT$  values also exceed any known metallic systems, including constantan, the nickel-copper alloy used for decades in thermocouples.

In this work we present results of *ab-initio* calculations based on the Density Functional Theory to investigate the electronic structure and transport properties of  $\text{Ni}_x\text{Au}_{1-x}$ . Electronic densities of states and Bloch spectral functions of  $\text{Ni}_x\text{Au}_{1-x}$  are obtained using the KKR-CPA method (Korringa-Kohn-Rostoker with coherent potential approximation). Calculations were performed in fully-relativistic manner, that is spin-orbit coupling was included. Energy dependent transport function was obtained with the Kubo-Greenwood formalism and for the thermopower full Fermi integrals were used. We show that resonant scattering determines the transport properties in this system and compare them to the case of Cu-Ni alloy.

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## Atomistic Simulations of Laser-based Powder Bed Fusion

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Laser-based powder bed fusion is a new technique to produce objects by additive manufacturing, in contrast to ordinary subtractive manufacturing processes like drilling, milling, cutting. Applications of additive technologies continue to demand an improvement in quality and reproducibility. Using simulations and physical models we are able to better understand the root causes for defects and may be able to derivate actions for defect avoidance. This paper presents a novel approach to the simulation of additive manufacturing using molecular dynamics simulations. By solving Newtons equations of motion iteratively we are able to yield the time evolution of the system and can simulate the melting of single particles or particle clusters. The biggest challenge to the simulations are the scales: although we use multi-million atom systems and run “long” simulations we have to scale parameters like particle size, laser power, power density, scanning speed, laser focus diameter and gravity.

Using parameter studies for scanning speed and laser power while also including the influence of protective argon gas, different inclusion defects in pure aluminum particles are shown. The simulation of powder beds formed by spheres of different sizes show holes which vanish if filled with vacuum but persist if the simulation box is filled with protective gas allowing insight into the defect formation. Recrystallization in a box filled with a bimodal distribution of aluminum particles has been observed. Additionally, different configurations of binary materials made of aluminum and titanium have also been simulated: the study compares spheres formed by a core of aluminum and an outer shell of titanium or vice versa, and homogenous spheres of a TiAl alloy.

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[3] K. Vietz, J. Schmid, J. Roth, Molecular Dynamics Simulation of Laser-based Powder Bed Fusion, in *High Performance Computing in Science and Engineering '23*, eds. W.E. Nagel, D.B. Kröner, M.M. Resch, Springer (2023) in print



## **AlCoFeNiCu<sub>x</sub> (x = 0.6 – 3.0) and (GaNi)<sub>x</sub>CoCrFe (x = 0.4 – 1.6) zero-magnetostriction magnetically soft high-entropy alloys for supersilent AC magnetic applications**

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AlCoFeNiCu<sub>x</sub> (x = 0.6 – 3.0) and (GaNi)<sub>x</sub>CoCrFe (x = 0.4 – 1.6) high-entropy alloys (HEAs) are a new class of magnetically soft alloys that demonstrate zero-magnetostriction and potential for use in supersilent AC magnetic applications. Investigated materials have desirable mechanical and magnetic properties, making them suitable for use in aerospace, automotive, and electrical engineering applications.

A comprehensive analysis of the magnetic properties of AlCoFeNiCu<sub>x</sub> HEAs was published in "Advanced Materials Interfaces" [1], while the study of (GaNi)<sub>x</sub>CoCrFe (x = 0.4 – 1.6) is still work in progress. The study of AlCoFeNiCu<sub>x</sub> alloys showed that the addition of Cu to the AlCoFeNi system improves magnetic properties, including increased magnetic permeability, saturation, and anisotropy. At a specific concentration of Cu, the material exhibits zero magnetostriction, making it ideal for low-noise applications in motors and generators. The alloys' high thermal stability and ability to maintain magnetic properties over a wide temperature range were also demonstrated.

The microstructures of the AlCoFeNiCu<sub>x</sub> (x = 0.6 – 3.0) alloys were analyzed and found to contribute to their superior magnetic properties, with a three-phase structure leading to zero magnetostriction. The magnetostrictions of individual phases compensate each other, with some having positive values and other negative values.

In conclusion, our study evaluates the magnetic properties and potential applications of AlCoFeNiCu<sub>x</sub> HEAs for supersilent devices. The results highlight the alloys' exceptional magnetic properties, high thermal stability, and unique microstructures, making them suitable for low-noise industrial applications. Similar properties are expected for the (GaNi)<sub>x</sub>CoCrFe (x = 0.4 – 1.6) high-entropy alloys.

[1] J. Luzar, P. Priputen, S. Vrtnik, et al., Adv. Mater. Interfaces 2201535 (2022).



## Magnetic Properties of Quasiperiodic Artificial Spin-Ice Tilings Fabricated with Nanolithography

Liam, Chandler<sup>1,\*</sup>, Oliver Barker<sup>1</sup>, Connor Fields<sup>2</sup>, Tyler James<sup>2</sup>, Liam O'Brien<sup>1</sup>, Alexander Wright<sup>1</sup>, Samuel Coates<sup>1</sup>, Ron Lifshitz<sup>3</sup>, Phillip Moriarty<sup>2</sup>, Ronan McGrath<sup>1</sup>, Hem Raj Sharma<sup>1</sup>

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Thin films deposited on quasicrystal surfaces have revealed intriguing novel configurations with quasiperiodic order [1,2]. However, investigating fundamental interactions such as magnetic moment ordering in such systems is limited by defects and the sensitivity limits of atomic probes in UHV.

In this work, these challenges are overcome by fabricating mesoscopic 2D quasiperiodic tilings of ferromagnetic metallic alloys with thermal scanning probe lithography. Ferromagnetic moments energetically arrange into mesoscopic domains with parallel spin along the long axis, when isolated, long single-domain “islands” produce a playground of macroscopic magnetic structure interactions known as artificial spin-ice [3]. Ordered arrays, including hexagonal, square, and the 5-fold Penrose tiling, have been investigated to probe emergent ordering in such systems [4]. This work uses micromagnetic simulations and magnetic microscopy methods to investigate the 8-fold Ammann-Beenker tiling, unique for its evenly divisible rotational order which should aid ground state formation. We aim to better understand high-energy domain wall formation, how a degenerate ground state nucleates, and to what extent quasiperiodic order forbids a unique ground state.

**Acknowledgements:** We acknowledge the Leverhulme Trust and UoL EPSRC DTA scheme for financial support.

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## New ToF ERDA experimental setup at the Slovak University of Technology in Bratislava for the characterisation of hydrogen storage and battery materials

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Global de-carbonization strategies rely to a great extent on light-element based materials such as lithium or hydrogen as the energy carrying/storage medium. Battery research pursues higher energy density and capacity, increased lifespan, faster charging, safety and thermal management, more abundant resources and less material consumption[1,2]. To achieve these objectives it is crucial to thoroughly understand and know the location, phase, and concentration of elements within various components of the battery such as electrodes, separators, electrolytes, encapsulation etc. In the case of hydrogen, development of effective storage and transportation as well as hydrogen burning systems hinges on gaining reliable insights into the interaction of hydrogen and the structural, and functional materials in these systems. This involves diffusion, hydrogen penetration into the respective material which could lead to hydrogen cracking on one hand and effectivity of hydrogen capture on the other [3,4].

Recently a new Time-of-Flight Elastic Recoil Detection Analysis (ToF ERDA) experimental setup was commissioned at the Slovak University of Technology in Bratislava. The system expands the capabilities of the 6 MV tandem ion accelerator system by the ability for quantitative characterisation of light elements, hydrogen or lithium down to ppm levels including depth profiling of layers up to 1  $\mu\text{m}$ . The system is based on the Jyväskylä spectrometer design [5] and is expected to deliver depth resolutions down to nm, which is expected to contribute to the understanding of the degrading mechanisms in battery electrode materials, hydrogen storage effectivity and provide supporting data to other methods for phase identification in the investigated materials.

In-situ and in-operando characterisation is envisaged, where the migration of ions (e.g. lithium) during charging/discharging cycles and diffusion phenomena can be assessed. We present the capabilities of the system together with first measurement results on various metallic compounds.

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# **POSTER SESSION**

**28<sup>th</sup> November 2023 late afternoon**





## The Ce-Au-X (X = Al, Si, Ga, Ge, Sn) ternary phase equilibrium around the quasicrystalline composition

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Since the discovery of the stable binary Cd<sub>5,7</sub>Yb [1] and Cd<sub>5,7</sub>Ca [2] icosahedral quasicrystals (QCs), there has been an increasing interest in these quasicrystalline structures and their approximants. These quasicrystalline phases, known as Tsai-type QCs, and their related approximants (1/1: Cd<sub>6</sub>Yb Type, SG: *Im-3*, and 2/1: Cd<sub>76</sub>Yb<sub>13</sub> SG: *Pa-3*) are built from similar clusters consisting of concentric shells of disordered tetrahedra, dodecahedra, icosahedra, icosidodecahedra and defected triacontahedra from the inside out.

Similar approximant structures, called 1/1 QC approximant, crystallizing with the body centered space group *Im-3*, have been reported in ternary systems like RE-Au-X [3-5], RE-Ag-X [6] with RE = Rare earth, Ca [7] or Na [8] and X a metalloid element or in Sc-Mg-Zn system [9]. All these systems have similar clusters but differ significantly by their respective composition. For example, gold systems usually crystallize with composition around RE<sub>15</sub>Au<sub>65</sub>X<sub>20</sub>, for silver it is approximately around RE<sub>20</sub>Ag<sub>40</sub>In<sub>40</sub> and for the Sc-Mg-Zn the 1/1 composition is Sc<sub>14,4</sub>Mg<sub>0,8</sub>Zn<sub>84,8</sub> [9]. The same behavior can be observed for the 2/1 approximant.

In this framework, we will concentrate here on Ce-Au-X systems, with X = Al, Si, Ga, Ge and Sn. The paper will report the structural characterization of both 1/1 and 2/1 approximants in these ternary systems showing their equilibrium relationship with the surrounding ternary phases. These investigations have been performed using powder XRD, microprobe analysis using X-ray energy dispersive analyses (EDAX), and single crystal analyses.

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## Novel open-framework PdO<sub>2</sub> structures predicted from first-principle calculations

P2

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Palladium is an important catalyst in many catalytic reactions with diversity of technological applications. Apart from the pure metal, catalytic activity is being increasingly attributed also to palladium oxides, which however remain poorly characterized. The only thoroughly studied and technologically exploited palladium oxide phase is PdO, while less attention has been paid to PdO<sub>2</sub>. Formation of only one polymorph with rutile structure was reported for the latter [1]. In our computational study based on Density Functional Theory, we demonstrate that PdO<sub>2</sub> exhibits the ability to assume a diverse range of open-framework structures capable of accommodating a wide variety of intercalated species. [2]. Importantly, their thermodynamical stabilities compete with that of the rutile type. We have thoroughly examined the energetics, crystal structure, electronic and phonon structure, mechanical stability and elastic properties of these predicted framework using several exchange-correlation functionals. Our results reveal similar polymorphism and energetics as is known for intensively researched MnO<sub>2</sub> open-framework structures [3-5]. The open frameworks offer wide possibilities for selective synthesis and modulation of properties by the intercalates, thus opening new possibilities for technological applications of PdO<sub>2</sub>.

### Acknowledgement:

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## Study of novel Ni-O phase Ni<sub>2</sub>O<sub>5</sub> from first principles

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Pentoxides of the fifth group elements (V<sub>2</sub>O<sub>5</sub>, Nb<sub>2</sub>O<sub>5</sub>, Ta<sub>2</sub>O<sub>5</sub>) exhibit a diverse range of structures, offering various potential applications. However, pentoxides of transition metals beyond the fifth group, such as our focus Ni<sub>2</sub>O<sub>5</sub>, have received limited or none attention. Ni<sub>2</sub>O<sub>5</sub> represents an intriguing, yet undiscovered phase, and our research seeks to predict its crystal structure and associated properties through the application of Density Functional Theory (DFT) and evolutionary algorithms (EA). We investigated the possibility of introducing nickel as the transition metal into well-studied M<sub>2</sub>O<sub>5</sub> structures and we have utilized DFT and EA to explore the most stable structures and their properties. Our study aims to expand our comprehension of the potential uses of novel nickel oxide materials.

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Scientific Grant Agency of the Slovak Republic, grant No. VG 1/0223/19;

The Slovak Research and Development Agency, grant No. APVV-18-0168;

The Slovak Research and Development Agency, grant No. APVV-20-0220;

Aurel supercomputing infrastructure in CC of Slovak Academy of Sciences acquired in projects ITMS 26230120002 and 26210120002 funded by ERDF;

PRACE FENIX Project fnxp070004 at TGCC high performance computing infrastructure, France.



## Superconductivity in gold nanostructures with niobium thin film percolating patterns

P4

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We studied superconductivity in gold nanostructures on which niobium thin film percolating patterns were deposited, as shown in Fig. 1.

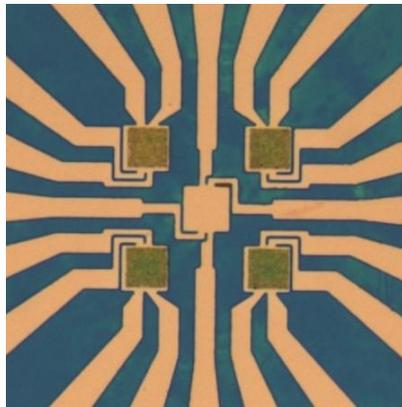


FIG. 1: Gold nanostructure with four Nb samples. Size of Nb samples is  $20 \times 20 \mu\text{m}$ .

We used two nanostructures (one is shown in Fig. 1.), each with four Nb samples. Samples are characterized by the percolation parameter  $p$ . The nanostructures were produced using UV lithography and gold was deposited by thermal evaporation. Matlab was used to create percolating patterns, which were written using e-beam lithography and niobium was deposited using DC sputtering.

We measured the temperature dependence of electrical resistivity, with and without the applied magnetic field, to investigate the metal-superconductor transition. We also measured the  $I$ - $V$  characteristics. All samples are superconducting with transition temperatures ( $T_C$ ) in the range 3 K – 5 K. Metal-superconductor transition curves exhibit anomalies which we attribute to the proximity effect. Using the change of  $T_C$  with the applied field, we extrapolated the values of upper critical field at 0 K  $H_{C2}(0)$  and of coherence length  $\xi(0)$ . Furthermore, a scaling analysis was carried out, by variation of magnetic field, from which we obtained the values of products of critical exponents and determined the universality classes of the samples [1].

In future research, we plan to carry out measurements in a wider  $p$  range, so that we can determine the critical value of  $p$  at which the superconducting transition occurs. Then, also a scaling analysis by variation of the percolation parameter could be performed.

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## Magnetotransport of a single crystal rutile TiO<sub>2</sub>

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Polaronic materials are an active topic in multidisciplinary field of physics, chemistry and materials science. Polarons play an important role in a range of physical properties such as charge transport, surface reactivity and magnetoresistance. [1]

In this study, we present the magnetic field dependence of the electrical resistivity of a polaronic material, a single crystal rutile TiO<sub>2</sub>, which is hardly found in the literature. The electrical resistivity has a minimum at 30 K and increases by six orders of magnitude when cooled down to 2 K. In the magnetic field, the electrical resistivity increases especially at low temperatures.

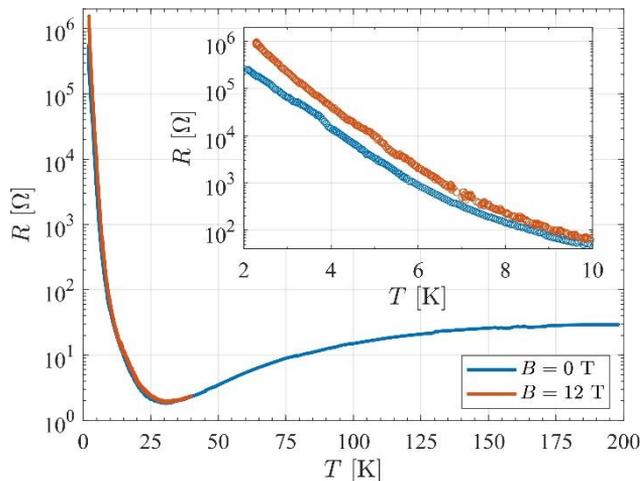


Figure 1. Temperature dependence of the resistivity of rutile TiO<sub>2</sub> single crystal for 0 T and 12 T.

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## Experimental simulation of the effect of transmutation helium on structural steels for nuclear applications

P6

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For materials used in advanced nuclear reactors, both fission and fusion, high levels of transmutation helium pose a significant challenge. Accumulation of this transmutation product stabilizes vacancy-type defects and leads to the formation of helium bubbles resulting in swelling and embrittlement of the material [1]. While most of the research on fundamental aspects like defect evolution and void swelling is performed at the nanoscale, our research focuses on the bulk properties of these materials and their practical applications in engineering.

We irradiated 6 structural steels designed for use in demanding radiation environments, namely SIMP, Eurofer97, PM2000, ODS Eurofer, SS 310S, and 800H by employing helium ion irradiation with energies ranging from 17 MeV down to 1 MeV, gradually decrementing the ion-beam energy to create a uniform "box-profile" of 1000 appm helium concentration [2]. As a result, we achieved a 65  $\mu\text{m}$  thick quasi-homogeneous irradiated layer, which enables to perform micromechanical testing and assessment of engineering relevant (bulk) material properties as well as the application of conventional positron annihilation spectroscopy utilizing radioisotope sources such as <sup>22</sup>Na positron source. This provides positrons with a continuous spectrum of energies up to 540 keV, which corresponds to ~ 85-90% positron stopping in 65  $\mu\text{m}$  [3]. In this contribution we present first results from positron annihilation lifetime spectroscopy and nanoindentation analysis.

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## NEUTRON DIFFRACTION STUDY OF PLASTIC DEFORMATION MECHANISMS IN AZ31 MAGNESIUM ALLOY

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Measurements of stress distribution in a polycrystalline material provide important information about the mechanisms of plastic deformation occurring at the scale of polycrystalline grains. Experimental methodology presented in this work is based on neutron diffraction experiment and it allows to determine stresses localised in grains during mechanical tests. The diffraction measurements were done during tensile test performed at the HK9 strain diffractometer (NPI, Rez, Czech Republic) using 2 $\theta$ -dispersion method (neutron diffraction). The lattice strains in AZ31 Mg-alloy were measured in-situ and the Crystallite Group Method (CGM) [1,2] was used to determine the evolution of the grain stresses for specific orientations of crystallites [3]. On the basis of the grain stress evolution a large difference in work hardening was found for crystallites having different lattice orientations.

Next, the variation of the Resolved Shear Stresses (RSS) were determined and their critical (CRSS) values were found for different slip systems. Results showed, that the basal system does not lead to significant macroscopic plastic deformation (activation of basal system occurs for non-preferred crystal orientations), important macroscopic plastic deformation occurs when the non-basal systems are activated (for significantly higher applied stress).

The mechanisms of elastic-plastic deformation was also simulated by Elastic-Plastic Self-Consistent model (EPSC). The value of CRSS for a basal slip system and adjusted set of CRSS values for non-basal slip systems determined with the help of the modified EPSC model agree with those obtained from a direct method. The predictions of the model agree with experiment if significant plastic accommodation is introduced for the plastically deformed grains [3].

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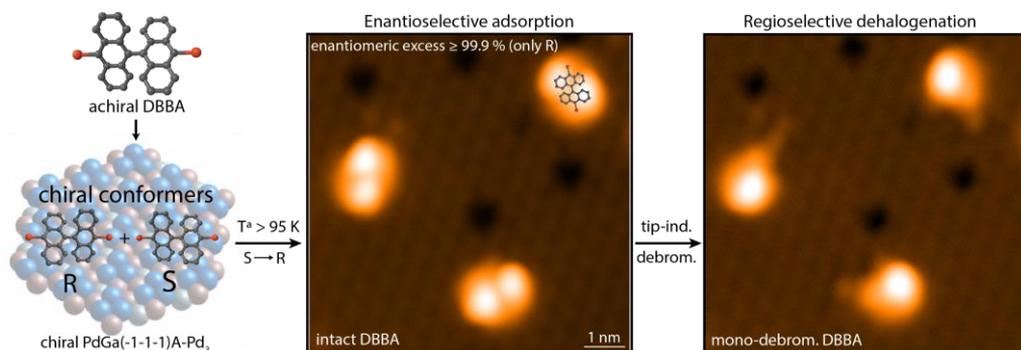
## Asymmetric adsorption and bond selectivity on chiral PdGa surfaces

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The unconventional chiral-crystal structure of intermetallic PdGa substrates provide them with intriguing properties from the point of view of asymmetric heterogeneous catalysis. They combine a valence electronic structure similar to copper with well-ordered, chiral local atomic structures at the different possible PdGa bulk truncated surfaces [1]. In this work, we make use of PdGa(-1-1-1) which features periodically ordered Pd trimers in the terminating layer. This particular surface structure cannot only transmit its innate chirality either to different adsorbates and the on-surface reactions which the former may subsequently undergo [2], but also act as 'platform' to host fundamental quantum phenomena as highly direction molecular tunneling motion [3].



**Figure 1.** a) 3D-modeled scheme illustrating the temperature-dependent enantioselective adsorption. b,c) STM images (50 mV, 100 pA) of DBBA molecules on the Pd<sub>3</sub>-terminated PdGa(-1-1-1) exclusively featuring the energetically favored conformer R in its three predominant orientations (b) before and (c) after regiospecific tip-induced debromination.

In our presentation, we will discuss the adsorption and debromination characteristics the well-known achiral di-bromo-bi-anthracene molecule (DBBA) which upon cold-deposition renders two different adsorption-induced chiral configurations. Given the chiral nature of the surface, one molecular conformation is energetically favored and, as a result, above 95K, the system transitions from a racemic mixture to a >99% enantio-pure adsorption state through a molecular reconfiguration process. Very remarkably, this now unique chiral adsorption configuration features highly different debromination characteristics between its two halogenated positions resulting into a robust tip-induced regiospecificity. Furthermore, the temperature-induced formation of chiral graphene nanoribbons is addressed. Our results highlight the auspicious role of chiral intermetallic PdGa substrates in the development of



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innovative asymmetric heterogeneous catalytic methods and the production of chiral-enriched nanostructures by on-surface synthesis strategies.

Support by the Swiss National Science Foundation under the grants 200021-129511 and 200021-159690 is gratefully acknowledged.

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[3] S. Stolz *et al. PNAS* **117**, 14838-14842 (2020).



## Martensitic phase transition in epitaxial Ni–Mn–Ga magnetic shape memory thin films: a surface science perspective

P9

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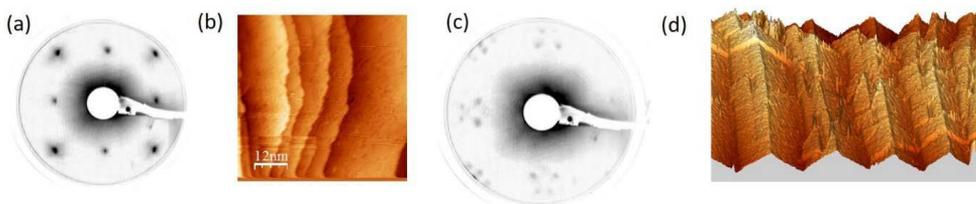
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Ferromagnetic shape memory (FSM) Heusler compounds are a class of “smart materials”, i.e. materials with multifunctional properties that can be activated through an external stimulus [1]. The prototype of FSM Heuslers is the Ni<sub>2</sub>MnGa intermetallic, because it shows the largest magnetic shape memory effect obtained so far. The key point at the heart of these externally driven physical changes and multifunctionality is a reversible martensitic transformation combined with a strong magnetostructural coupling. There is a strong interest in the basic physics of Ni–Mn–Ga ferromagnetic shape memory alloy because of its potential as a functional material with large magnetic field induced strain, as an energy material with giant magnetocaloric effect and as a magnetic sensor with large negative magnetoresistance.

Here we report first results on the surface of an epitaxial Ni-Mn-Ga thin film grown on MgO(001) by RF sputtering technique at elevated temperature (623 K) [2]. We use scanning tunnelling microscopy (STM) imaging, low-energy electron diffraction (LEED), x-ray photoemission spectroscopy (XPS) and scanning electron microscopy (SEM) to study the structural, chemical and microstructural changes occurring across the phase transition between the high temperature austenite with L2<sub>1</sub> structure and the low temperature martensite with seven-fold modulated monoclinic structure (Fig.1).



**Figure 1:** LEED patterns and STM images of the austenite (a,b) and the martensite (c,d) phases.

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## Influence of RF Sputtering Parameters on Hydrogen Content in Thin PdO Films by ToF-ERDA

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In this research, we have systematically deposited thin PdOx films via RF sputtering of Pd wire in a range of gas environments, including inert and oxidizing atmospheres. Our investigation delves into the critical factors influencing these thin films, specifically emphasizing the hydrogen content within the layers. The experimental parameters explored encompass oxygen-to-argon ratios, discharge power settings and pressure levels varying between  $5 \times 10^{-3}$  to  $5 \times 10^{-2}$  mbar.

In order to gain a comprehensive understanding of the films, we utilized advanced analytical methods, X-ray photoelectron spectroscopy, Scanning electron microscopy and Time of Flight Elastic Recoil Detection Analysis.

These methods not only facilitated the assessment of elemental composition and detection of impurities but also allowed for the precise determination of thickness of films, deposition rates, composition and chemical state.

Of particular importance is the inherent propensity of PdO to bond with hydrogen, aligning with Palladium's well-recognized role as a catalyst in various applications, including H<sub>2</sub>O<sub>2</sub> synthesis and hydrogen detection. Thus, the investigation of hydrogen content within these PdOx layers assumes paramount significance, holding promise for enhancing their catalytic performance and expanding their utility in catalytic processes and hydrogen-related technologies.



## Growth of crystalline CoCrFeNi high-entropy alloy thin films on LaAlO<sub>3</sub> by magnetron sputtering

P11

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Multicomponent alloys of at least four elements with near equimolar percentage were first reported and investigated by Cantor *et al.* [1] and Yeh *et al.* [2] in 2004 and are nowadays often referred to as High-Entropy Alloys (HEAs) [3]. This composition is expected to support the formation of single-phase solid solutions, which lead to extensive research on the mechanical properties of HEAs in the past decades, but surface physics are barely investigated so far. Recently, we have demonstrated the formation of crystalline thin films of CoCrFeNi via magnetron sputtering from homemade targets on MgO (100) single crystal substrates [4]. The single crystal character of the films and its epitaxial relation to the substrate were confirmed by X-ray diffraction (XRD) and transmission electron microscopy (TEM). Following a proper UHV surface treatment, the structural and electronic behaviour is accessible by means of low energy electron diffraction (LEED) and angle resolved photoelectron spectroscopy (ARPES).

In the present study, the proof of principle for this method of crystal fabrication is demonstrated by deposition of CoCrFeNi on LaAlO<sub>3</sub> (LAO) substrates. Access to surface studies on different CoCrFeNi crystal planes is achieved by the variation of the substrates surface orientation which determines the HEA growth direction. Since the lattice constants of LAO and CoCrFeNi are very similar, the occurrence of planar defects, which were observed more frequently on MgO, could be significantly reduced.

[1] Cantor *et al.*, Mater. Sci. Eng. A, 213, **375-377**, (2004)

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## Magnetocaloric properties of single-crystalline $\text{Eu}_5\text{In}_2\text{Sb}_6$

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The Zintl phase  $\text{Eu}_5\text{In}_2\text{Sb}_6$  crystallizes in the orthorhombic  $\text{Ca}_5\text{Ga}_2\text{As}_6$ -type structure (nonsymmorphic space group *Pbam*, no. 55). It orders antiferromagnetically (AFM) at  $T_{\text{N1}} \approx 14.0$  K and undergoes another AFM phase transition at  $T_{\text{N2}} \approx 7.1$  K. The compound exhibits insulator-like electrical transport. Above  $T_{\text{N1}}$ , it displays colossal magnetoresistance (CMR) accompanied by an anomalous Hall component. Due to fairly low thermal conductivity that is a consequence of complex bonding environment,  $\text{Eu}_5\text{In}_2\text{Sb}_6$  shows superior thermoelectric performance.

In this study, we determined the magnetocaloric properties of  $\text{Eu}_5\text{In}_2\text{Sb}_6$  in a wide range of temperature and within different magnetic field intervals. Single crystals of the compound were grown using In-flux technique. The magnetocaloric effect (MCE) was studied in magnetic fields aligned within the crystallographic *ab*-plane and along the *c*-axis. From the analysis of Arrott plots we concluded that the AFM transitions are of the first-order type. The compound displayed both normal and inverse MCE, and furthermore, owing to its substantial anisotropy, a rotational MCE was found. Notably, for conventional MCE, the maximum value of isothermal entropy change  $\Delta S_{\text{m}}$  was  $-4.7(1) \text{ J kg}^{-1} \text{ K}^{-1}$  at  $15(1) \text{ K}$  for a magnetic field change  $\Delta B$  of 5 T, regardless the field orientation. The relative cooling power (RCP) was found similar for both field directions, equal to  $81(1) \text{ J kg}^{-1} (\Delta B = 5 \text{ T})$ . The largest rotational MCE was observed near 11 K, with maximum  $\Delta S_{\text{R}}$  value of  $2.4(1) \text{ J kg}^{-1} \text{ K}^{-1}$  and  $\text{RCP} = 17.5(6) \text{ J kg}^{-1}$  for  $\Delta B = 4 \text{ T}$ . The practical attractiveness of  $\text{Eu}_5\text{In}_2\text{Sb}_6$  is enhanced by the coexistence of normal, inverse and rotational MCE.

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## Short-range order effects in paramagnetic states of single-crystalline $\text{EuIn}_2\text{P}_2$ and $\text{EuIn}_2\text{As}_2$

P13

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The compounds  $\text{EuIn}_2\text{P}_2$  and  $\text{EuIn}_2\text{As}_2$  crystalize with hexagonal unit cells (space group  $P6_3/mmc$ ). The phosphide orders magnetically at  $T_C = 24$  K, with the Eu magnetic moments aligned ferromagnetically within the  $ab$  plane but tilted alternately along the  $c$ -axis. Below  $T_N = 16.1$  K,  $\text{EuIn}_2\text{As}_2$  exhibits an antiferromagnetic arrangement of the adjacent  $ab$  planes, keeping an in-plane ferromagnetic alignment of the Eu magnetic moments [1-3].

In the paramagnetic state, the thermodynamic and electrical transport properties of both materials are dominated by short-range magnetic interactions, which manifest themselves as: (i) strongly anisotropic magnetic susceptibility even far above  $T_C/T_N$ , (ii) activation-type resistivity behaviour that can be well described in terms of variable-range hopping transport, (iii) negative magnetoresistance that varies quadratically with magnetic field strength as well as with reduced magnetization [4], (iv) transverse magnetoresistance describable by models appropriate for localized magnetism.

*This study was supported by the National Science Centre (Poland) under grant 2021/41/B/ST3/01141.*

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- [4] Y. Zhang, et al., Phys. Rev. B 101, 205126 (2020)



## The appearance of anomalous Hall effect in $\text{EuCd}_2\text{As}_2$ above ordering temperature

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Weyl semimetals have garnered significant attention owing to their wide array of exotic properties predicted by theoretical frameworks. They serve as an elegant illustration of the profound connection between condensed matter and high-energy physics, primarily due to their low-energy excitations known as Weyl fermions, which are massless particles obeying the Weyl equation. These materials exhibit linear dispersion in their energy bands near specific points called Dirac or Weyl points, akin to the three-dimensional counterpart of graphene. The remarkable mobility of charged Weyl fermions holds great promise for applications in electronics and computing.

As for the layered antiferromagnet,  $\text{EuCd}_2\text{As}_2$ , it was initially considered a member of the Weyl semimetal category. However, recent studies conducted by our team with collaborators do not substantiate this assertion. Our findings reveal that  $\text{EuCd}_2\text{As}_2$  can display either insulating or metallic behavior contingent on the specific synthesis method employed. Within the insulating phase, we have identified a notable anomalous contribution to the Hall effect, possibly attributable to the formation of magnetic polarons. Currently, we cannot exclude the possibility of a two-band contribution to the Hall signal.



## Investigation of Transport and Magnetic Properties of Intercalated TMDs

P15

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Transition metal dichalcogenides (TMDs) are layered materials that, due to their reduced dimensionality, host interesting phases such as charge density waves (CDW) and superconductivity. Intercalation by first-row transition metals offers the possibility of fine-tuning magnetic and electronic properties [1]. We synthesized high-quality single crystals of  $\text{Ni}_x\text{NbS}_2$  in a wide intercalation range of  $0.01 < x < 0.6$ , and stoichiometric  $\text{Co}_{1/3}\text{TaS}_2$ . In  $\text{Ni}_x\text{NbS}_2$ , we study the suppression of superconductivity and the development of the antiferromagnetic (AF) phase. We also investigate the effect of disorder on the magnetic ground state. It's interesting to notice that although both compounds order antiferromagnetically, a ferromagnetic component also exists indicating the presence of Dzyaloshinskii-Moriya interaction. ARPES study and experiments under hydrostatic and uniaxial pressure are currently underway to get a more comprehensive understanding of the ground state and its electronic structure [2,3].

### ACKNOWLEDGMENTS

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## Crystal structure study of non-centrosymmetric EuTGe<sub>3</sub> (T = Co, Rh, and Ir) under hydrostatic pressure

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Intermetallic EuTX<sub>3</sub> (T : transition metal, X = Si/Ge) forms a non-centrosymmetric BaNiSn<sub>3</sub>-type structure (space group *I4mm*). It has been attracting considerable attention due to complex magnetic structures and unique pressure phase diagram that potentially accommodates superconductivity under pressure [1,2]. Unlike Eu-compounds with the ThCr<sub>2</sub>Si<sub>2</sub>-type structure, detailed studies of pressure dependent structural changes in those with the BaNiSn<sub>3</sub>-type structure remain to be scarce. In order to study the pressure evolution of crystal structure, we performed synchrotron powder x-ray diffraction (XRD) as a function of pressure on EuTGe<sub>3</sub> (T=Co, Rh, Ir) at 300 K. The obtained lattice volume exhibited a smooth contraction without any symmetry changes in all compounds. From the equation of state fitting of the unit cell volume [3], we obtained the bulk modulus and the pressure derivative of the bulk modulus of all compounds. Our study also revealed an anisotropic compressibility between *a*- and *c*-axis. The axial ratio (*c/a*) increased by applying pressure and exhibited a slope change around 21 GPa in EuCoGe<sub>3</sub> [4], 15 GPa in EuRhGe<sub>3</sub> and 22 GPa in EuIrGe<sub>3</sub>. The pressure change of the *c/a* ratio seems to reflect changes in local environment, *e.g.* different pressure responses of bond lengths.

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## Electronic transport in intercalated 2H-NbS<sub>2</sub> modulated by magnetic 3d orbitals

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Layered compounds, due to their reduced dimensionality, are susceptible to different instabilities leading to realization of various, sometimes exotic, electronic phases. Their layered structure enables exfoliation and often intercalation, rendering them promising candidates for new electronic devices and applications. Transition-metal dichalcogenides (TMDs) are prominent members in this class of compounds. They support various charge density waves, metallic and semi metallic, superconducting and Mott insulating states. Intercalation with transition metal ions adds magnetic sublayers, which also show various magnetic ground states. Co<sub>1/3</sub>NbS<sub>2</sub> and Ni<sub>1/3</sub>NbS<sub>2</sub> both order antiferromagnetically below their respective ordering temperatures  $T_{N,Co} = 28$  K and  $T_{N,Ni} = 95$  K. However, while the complete suppression of magnetic order under pressure has been observed in Co<sub>1/3</sub>NbS<sub>2</sub> [1, 2], the magnetic ordering in Ni<sub>1/3</sub>NbS<sub>2</sub> behaves more robustly under pressure. The electronic transport anisotropy further demonstrates the differences between the roles that Co and Ni play upon intercalation. This difference is also shown in the electronic structure of two compounds, here explored through angle resolved emission spectroscopy (ARPES), ab initio electronic structure calculations and modeling [3, 4]. It is demonstrated that intercalated ions dominate the interlayer coupling. In the case of Co<sub>1/3</sub>NbS<sub>2</sub> we propose the “spin-valve” mechanism where the intercalated Co ions act as spin-selective electrical transport bridges between host layers.

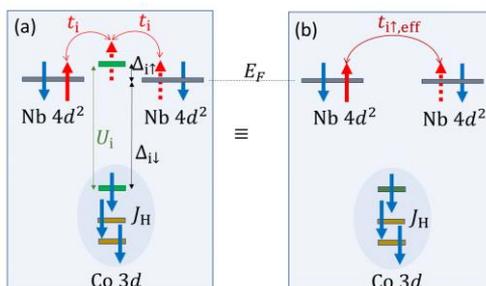


Figure 1. The figure illustrates electron hopping between two Nb 4d orbitals of neighboring NbS<sub>2</sub> layers, facilitated by the Co 3d<sub>z<sup>2</sup></sub> orbitals (depicted as green bars) of the intercalated cobalt atom.

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## Synthesis, characterization, and magnetic studies of Mn<sub>2</sub>P

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Transition metal phosphides are a class of materials with diverse applications in catalysis, energy storage, and electronic devices [1-3]. This work focuses on antiferromagnetic Mn<sub>2</sub>P with Néel temperature ( $T_N$ ) ~103 K [4]. Mn<sub>2</sub>P crystallizes in a non-centrosymmetric hexagonal structure (space group:  $P\bar{6}2m$ ). Mn atoms occupy two inequivalent tetrahedral and pyramidal sites which carry small and large moments, respectively [4, 5]. Although Mn<sub>2</sub>P has been known for decades, the reported magnetic structure varies depending on the experimental methods [4, 6]. Moreover, inconsistent temperature behaviors of electrical resistivity and two order of magnitude different residual resistivity have been reported depending on crystals [7]. In order to investigate the intrinsic magnetic and electric properties of Mn<sub>2</sub>P, high quality single crystals are required. Following that, we have grown single crystals of Mn<sub>2</sub>P by Sn-flux method. Chemical composition and crystal structure were studied by energy dispersive x-ray spectroscopy and powder x-ray diffraction. The chemical composition of the grown crystal is determined as Mn<sub>2</sub>P. We also measured the magnetic susceptibility curve and its field dependence on the grown Mn<sub>2</sub>P single crystals. The grown crystals exhibit an antiferromagnetic transition at  $T_N = 104$  K which is in a good agreement with previous studies [7, 8]. A shoulder like feature is seen in the susceptibility curve around 50 K. With an increase in the external magnetic field, the shoulder like feature becomes more prominent. The result implies a presence of meta-magnetic transition.

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## Phase separation and recovery in ferritic oxide dispersion strengthened steels

P19

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Oxide dispersion strengthened (ODS) alloys are promising structural materials for high temperature application and for next generation fission/fusion reactor applications. They offer enhanced high temperature creep strength in combination with good irradiation resistance. High chromium ferritic ODS steels show also improved corrosion resistance and allow extending the operation temperature beyond 650 °C. However, high chromium steels may suffer from hardening embrittlement, which is attributed to the phase separation into Fe-rich  $\alpha$  and Cr-rich  $\alpha'$  phases forming during thermal ageing of the material at intermediate temperatures. Presence of  $\alpha'$  results in an increase of strength and ductile–brittle transition temperature, and a concomitant loss of ductility and corrosion resistance.

The  $\alpha - \alpha'$  phase separation and the dissolution of the  $\alpha'$  phase have been studied with thermoelectric power (TEP) and small-angle neutron scattering (SANS) measurements in recrystallized PM2000, MA956 and ODM751 ODS steels. Nanometric precipitation of  $\alpha'$  phase was quantified in terms of its volume fractions and precipitate sizes after 1000 hours ageing at 475 °C. A good correlation between the micro-hardness, thermoelectric power and precipitate volume fraction measured by SANS was established. The embrittlement of the aged material was evident from the tensile and impact tests. The ageing temperature of 650 °C was outside of the miscibility gap for both materials therefore  $\alpha'$  phase formation was not detected. For samples previously aged at 475 °C, further ageing at 650 °C resulted in complete dissolution of the  $\alpha'$  phase. Both non-destructive techniques applied confirmed the dissolution. SANS found to be suitable technique for studying the kinetics of the recovery.



## Investigating Ga-Sb-Pd Intermetallic Compounds as Catalysts for the Semi-Hydrogenation of Acetylene

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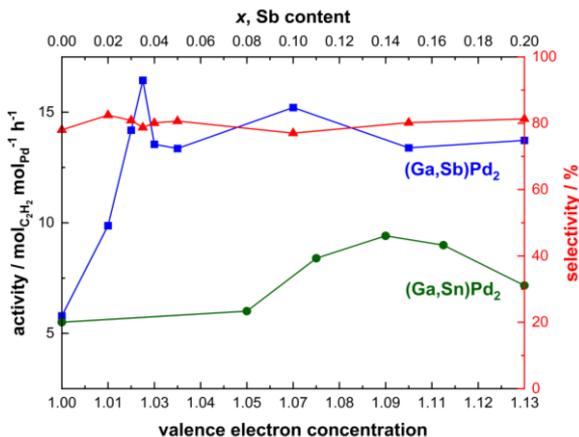
**Introduction.** The semi-hydrogenation of acetylene is an important industrial process to remove traces of acetylene from the ethylene feed used to produce polyethylene.[1] Ga-Pd intermetallic compounds have been studied as catalysts in the semi-hydrogenation of acetylene and were found to exhibit high selectivities and high stability.[2] Substitution of gallium with another main-group element having a higher number of valence electrons results in compounds with different valence electron concentrations, thus the electronic influences in the semi-hydrogenation of acetylene can be studied. An example of this is the catalytic investigation on  $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$  ( $0 \leq x \leq 1$ ), where the maximum activity was observed at  $x = 0.28$ . [3] In this work, Ga (with three valence electrons) is replaced with Sb (five valence electrons) to reduce the substitution degree while still improving the activity. Intermetallic compounds  $\text{Ga}_{1-x}\text{Sb}_x\text{Pd}_2$  ( $0 \leq x \leq 0.2$ ) were synthesised, characterized and catalytically tested in the semi-hydrogenation of acetylene.

**Experimental.** Intermetallic compounds  $\text{Ga}_{1-x}\text{Sb}_x\text{Pd}_2$  ( $x = 0, 0.02, 0.03, 0.035, 0.04, 0.05, 0.1, 0.15, 0.2$ ) were synthesised in a high-frequency furnace and subsequently enclosed in evacuated quartz glass ampoules before being annealed at 900 °C for three weeks in a resistance oven. Samples were then characterized using metallography and powder X-ray diffraction. This was followed by catalytic tests on crushed samples in a quartz glass tube reactor (plug-flow type) using a gas phase composed of 0.5%  $\text{C}_2\text{H}_2$ , 5%  $\text{H}_2$ , 50%  $\text{C}_2\text{H}_4$ , 44.5% He at 200 °C and a total flow of 30 mL/min.

**Results and discussion.** X-ray diffraction as well as metallography resulted in single-phase samples for all compositions. Catalytic testing of these samples revealed that the maximum activity was  $16.44 \text{ mol}_{\text{acetylene}} \text{ mol}_{\text{Pd}}^{-1} \text{ h}^{-1}$  at  $x$  (Sb content) = 0.035. Selectivity towards ethylene was around 80% for all samples displaying high stability throughout the catalytic testing. The valence electron concentration (total number of valence electrons divided by total number of atoms) were calculated for the Sb and Sn containing samples using each atom's valence electron count (Ga = three, Sb = five, Pd = zero, and Sn = four). Since



**Fig 1.** Selectivity of  $\text{Ga}_{1-x}\text{Sb}_x\text{Pd}_2$  samples, and activity of  $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$  &  $\text{Ga}_{1-x}\text{Sb}_x\text{Pd}_2$  samples as a function of valence electron concentration and  $x$  (Sb content) (lines are guide to the eye)



the change of valence electron concentration has been doubled per atom for Sb compared to Sn, the highest catalytic activity is expected at half the Sb content ( $x = 0.14$ ). However, this is not observed and the highest catalytic activity is seen at  $x = 0.035$  (Figure 1).

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## Surprising Magnetism of Murunskite

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There are only two known families of high- $T_c$  superconductors, the cuprates and the iron pnictides. Murunskite ( $K_2FeCu_3S_4$ ) bridges them structurally and electronically. It is an insulator like the cuprate parent compounds, however, magnetically it is more similar to pnictides. Magnetic properties of murunskite single crystals are presented, based on neutron (fig 1b), Moessbauer, and XPS measurements. They are difficult to reconcile with a microscopic picture of localized magnetic moments residing on individual atoms. The ordered phase is antiferromagnetic with a nearly commensurate quarter-zone wave vector.

However, the only chemically identifiable magnetic atoms are iron, which are distributed at random over one-quarter of available crystallographic sites in 2D planes (Fig1a). The remainder are occupied by closed-shell copper.

Furthermore, the measured size of the moments exceeds that of a Fe 3+ ion, even though the majority of iron atoms are in the 2+ oxidation state. Finally, the material is a 0.8 eV-gap semiconductor with the same moments visible in a paramagnetic state above the AF transition temperature, making an interpretation in terms of a spin-density wave also questionable. A tentative picture of moments delocalized over a magnetic unit cell and mediated by polarized sulfur ligands is presented.

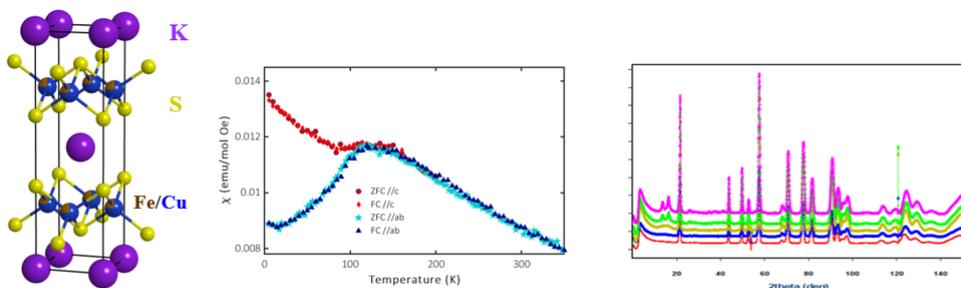


Fig1 (a) crystal structure of murunskite (b)magnetic susceptibility measurements and (c) Neutron powder diffraction.



## V-Ni intermetallic compounds in oxygen evolution reaction

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Alkaline water electrolysis is a reassuring method for emerging green hydrogen production with the aid of electricity obtained from renewable resources. Water oxidation half-reaction is assessed as the rate-limiting part of the water splitting due to its slow kinetics. During the last decade, Ni- and Co- containing binary compounds with well-defined crystal structures have attracted a tremendous attention [1,2]. Therefore, investigation of bulk well-characterized intermetallic compounds as electrocatalysts for the oxygen evolution reaction (OER) is a step forward in the future development and understanding of electrocatalyst for OER.

In the present study, electrochemical behaviour of selected V-Ni intermetallic compounds was investigated in comparison with elemental Ni. The working electrodes were prepared by solid-state synthesis followed by cutting into cylindrical shape with fine-polished surfaces. The prepared electrodes were extensively characterized to check purity and morphological properties before and after electrochemical experiments. Various electrochemical techniques were used to evaluate and compare OER behaviour in terms of their electrochemical activity and its stability over time. Results of recent findings in this study will be presented and discussed thoroughly.

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## Crystal Growth and Thermal Characterization of Intermetallic Compounds in the Yb-Au-Sn System

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The number of discovered intermetallic Tsai-type (YbCd<sub>6</sub>) icosahedral quasicrystals (iQC) has been continuously expanding and the substitution of Yb for other rare-earths (RE) and of Cd for binary mixtures with matching valence electron concentrations (VEC) have proven to be useful tools when investigating the formation conditions as to why these discrete structures represent thermodynamically favoured phases over periodic ones like the closely related approximant crystals (AC).<sup>[1]</sup>

We have studied the thermal behaviour of the intermetallic compounds in the Yb-Au-Sn system with a pseudo-binary approach, using eutectic Au<sub>71</sub>Sn<sub>29</sub> as one component and Yb as the other, mapping out the points of phase equilibria for the low Yb concentration region. Using a combination differential scanning calorimetry (DSC), solution growth experiments and bracketing by heat treating quenched melts, key features of the complex phase relations were unravelled, like the peritectic decomposition temperature of the iQC into the 2/1 AC. In addition, we detailed the synthesis of the iQC, 2/1 AC and a hexagonal phase of Gd<sub>14</sub>Ag<sub>51</sub> type structure. We discovered that the major phase from solution growth experiments using 4% – 6% at. Yb was Au<sub>4</sub>Yb with iQC presenting as the minor phase. The co-existence of iQC and 2/1 AC also seem to occur for a wider range of Yb concentrations than previously reported.<sup>[2]</sup> From energy dispersive x-ray spectroscopy, the compositions of the iQC and 2/1 AC were determined to be Yb<sub>12.9</sub>Au<sub>64.9</sub>Sn<sub>22.2</sub> and Yb<sub>13.9</sub>Au<sub>64.5</sub>Sn<sub>21.5</sub> respectively. From our bracketing experiments, the peritectic decomposition of iQC into 2/1 AC was estimated to be between 420°C-430°C, where a clear step was observed in the Yb content from EDS.

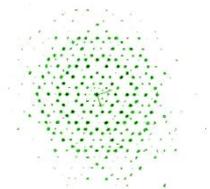


Figure 1- A single crystal x-ray diffractogram along the 5-fold rotational axis of an iQC grown from a mixture of 4% at. Yb and 96 % eutectic Au<sub>71</sub>Sn<sub>29</sub>.

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