

European C-MetAC

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

European C-MetAC Days 2022

November 21 – 24, 2022

Split, Croatia

Program

Dear participants of the ECMetAC Days 2022,

Welcome to Split, Croatia. It is our great pleasure to host such an important meeting, especially after two years of being online. We hope you will enjoy the meeting and your stay in Split.

The **venue** of ECMetAC Days is the campus of the University of Split, the "Three Faculties Building". Lunch will be organised in the University's restaurant (see picture below).



Accommodation is organized at the Park hotel, Hatzeov perivoj. Bus transfer is organized between the hotel and the campus.

To reach the campus by **public transportation**, enter "Kampus Split" as your destination on Google Maps. To plan your trip or buy tickets, you can download the application "Promet Split" (see QR codes below).



for Android



for iPhone

WiFi is available at the conference venue via *eduraom* and the “PMF” network (SSID: PMF, password: PMF1321.). The **online version of the program** is available at <https://projekti.pmfst.unist.hr/condmatlab/ECMetACDays2022/>



WiFi (PMF)



program online

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Marc de Boissieu (France)

Magdalena Wencka (Poland)

Julian Ledieu (France)

Schedule**Monday, November 21, 2022****HEA workshop, dedicated to the 65th anniversary of Prof. Janez Dolinšek**

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|-------|---|
| 13:00 | Ante Bilušić, Julian Ledieu, Magdalena Wencka: <i>opening</i> |
| 13:15 | Sheng Guo <i>Eutectic High-Entropy Alloys & Refractory High-Entropy Alloys: Opportunities and Challenges</i> |

Session 1: Structure and surfaces*Chair person: Sheng Guo*

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|-------|---|
| 14:00 | Anton Meden <i>Phase Identification and Quantification in High Entropy Alloys Using X-Ray Powder Diffraction</i> |
| 14:30 | Marc Armbrüster <i>HEAs in Catalysis - An Overview</i> |
| 15:00 | Andreja Jelen <i>Multi-phase structure of AlCoFeNiCu_x (x = 0.6 - 3.0) HEAs</i> |
| 15:20 | Coffee break (birthday cake & more...) |

Session 2: Physical properties*Chair person: Peter Gille*

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|-------|--|
| 16:20 | Jože Luzar <i>AlCoFeNiCu_x (x = 0.6 – 3.0) zero-magnetostriction magnetically soft high-entropy alloys</i> |
| 16:40 | Primož Koželj <i>Al_{0.5}TiZrPdCuNi in HEA vs metallic-glass form: How important is the crystallinity of HEAs for electronic transport?</i> |

Round table discussion and closing*Chair person: Magdalena Wencka*

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| 17:00 | Trends in development of high-entropy alloys |
| 17:20 | Janez Dolinšek, Julian Ledieu: closing |

Tuesday, November 22, 2022

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| 8:50 | opening |
| <i>Chair person: Ana Smontara, Zagreb</i> | |
| 9:00 | Emil Babić, Zagreb <i>Compositionally complex alloys: some problems and prospects</i> |
| 9:30 | Farid Labib, Tokyo <i>Emergence of long-range magnetic order from spin-glass state by tuning electron density in Ga-based 1/1 quasicrystal approximant</i> |
| 9:50 | Mario Novak, Zagreb <i>Nodal-line driven anomalous susceptibility in ZrSiS</i> |
| 10:10 | Neveen Singh Dhimi, Zagreb <i>Pressure evolution of electronic and crystal structures of EuTGe₃ (T = Co, Rh, Ir)</i> |
| 10:30 | Coffee break |
| <i>Chair person: Janez Dolinšek, Ljubljana</i> | |
| 11:00 | Holger Schwarz, Chemnitz <i>Growth of crystalline CoCrFeNi high-entropy alloy thin films by magnetron sputtering</i> |
| 11:20 | Priyanka Reddy, Zagreb <i>Murunskite: a bridge between cuprates and pnictides</i> |
| 11:40 | Josipa Šćurla, Split <i>High throughput in-vivo toxicity test of organo-metallic photovoltaic perovskites via micro fluidics on the C. elegans</i> |
| 12:00 | Željana Bonačić Lošić, Split <i>Collective plasmon modes of Dirac electrons in composite systems</i> |
| 12:20 | Marc de Boissieu, Grenoble <i>Thermal conductivity and lattice dynamics of aperiodic crystals</i> |
| 12:40 | Lunch |
| <i>Chair person: Janusz Tobola, Kraków</i> | |
| 14:30 | Silke Bühler Paschen, Vienna <i>Electronic topology driven by strong correlations</i> |
| 15:00 | Gaku Eguchi, Vienna <i>Specific heat of topological semimetals and insulators across the correlation spectrum</i> |
| 15:20 | Shovan Dan, Wrocław <i>Electrical transport in half-Heusler compound TmPdSb</i> |

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| 15:40 | Karan Singh, Wrocław <i>Anomalous electrical transport in EuZn_2Sb_2</i> |
| 16:00 | Coffee break |
| <i>Chair person: Silke Bühler Paschen, Vienna</i> | |
| 16:30 | Petar Popčević, Zagreb <i>Complexities of 2H-NbS_2 intercalations</i> |
| 16:50 | Eteri Svanidze, Dresden <i>Superconductivity and magnetism in complex mercury-based compounds</i> |
| 17:10 | Mitja Krnel, Dresden <i>Superconductivity in crystallographically disordered $\text{LaHg}_{6.4}$</i> |
| 17:30 | Diana Kirschbaum, Vienna <i>Effects of hydrostatic pressure on the Weyl-Kondo semimetal candidate CeRu_4Sn_6</i> |
| 17:50 | <i>Poster session</i> |
| 19:30 | <i>EB meeting</i> |

Wednesday, November 23, 2022

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| <i>Chair person: Peter Gille, München</i> | |
| 9:00 | Yuri Grin, Dresden <i>Chemical bonding and structural complexity</i> |
| 9:30 | Marc Armbrüster, Chemnitz <i>Catalytic and material complexity – In-Pt/In₂O₃ in methanol steam reforming</i> |
| 9:50 | Oytun Tiryaki, Chemnitz <i>Size-dependent methanol steam reforming investigated on unsupported ZnPd nanoparticles</i> |
| 10:10 | Fatma Aras, Dresden <i>Chemical behaviour of Mo₂TMB₂ (TM: Fe, Co, Ni) upon oxygen evolution reaction (OER)</i> |
| 10:30 | Coffee break |
| <i>Chair person: Émilie Gaudry, Nancy</i> | |
| 11:00 | Hem Raj Sharma, Liverpool <i>Surface properties of Ga₃Ni₂ and In₃Ni₂ intermetallic catalysts</i> |
| 11:20 | Alexis Front, Nancy <i>Structural stability of In-Pd intermetallic nanoalloys</i> |
| 11:40 | Thiago Trevizam Dorini, Nancy <i>Complex ultrathin oxide structures revealed by evolutionary computations : In_xO_y/PdIn(001)</i> |
| 12:00 | Oscar Shedwick, Liverpool <i>Surface composition & oxidation studies of Ga₃Ni₂ intermetallic alloy catalyst</i> |
| 12:40 | Lunch |
| <i>Chair person: Ronan McGrath, Liverpool</i> | |
| 14:30 | Marek Mihalkovič, Bratislava <i>Coherent interface between diamond and clathrate structures</i> |
| 15:00 | Émilie Gaudry, Nancy <i>Revealing the epitaxial interface between Al₁₃Fe₄ and Al₅Fe₂</i> |
| 15:20 | Wilfried Bajoun Mbajoun, Nancy <i>Structural investigation of the Ho-Au-Si (100) approximant surface</i> |
| 15:40 | Vincent Fournée, Nancy <i>Martensitic phase transition in epitaxial Ni–Mn–Ga magnetic shape memory thin films: a surface science perspective.</i> |

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| 16:00 | Coffee break |
| <i>Chair person: Eteri Svanidze, Dresden</i> | |
| 16:30 | Janusz Tobola, Kraków <i>Entropy engineering in materials for conversion energy (thermoelectrics & ion batteries)</i> |
| 16:50 | Monika Lužnik, Ljubljana <i>Size matters: a study on transport properties of type-I clathrate nanowires</i> |
| 17:10 | Laura Agnarelli, Dresden <i>Structural complexity in the apparently simple crystal structure of Be₂Ru</i> |
| 17:30 | Concluding remarks |
| 19:30 | Conference dinner |

Thursday, November 24, 2022

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| 8:15 | Science Board Meeting |
| 10:15 | Break |
| 10:30 - 12:00 | Governing Board Meeting and General Assembly |
| 13:00 - 17:00 | Katarzyna Gliszczyńska <i>Innovative Researcher: How to design a marketable bestseller PhD thesis</i> |

Poster presentations

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|------|---|
| P-1 | Alfahad Ahowd, Liverpool <i>Surface structure of In₃Ni₂ Inter-metallic compound</i> |
| P-2 | Mario Basletić, Zagreb <i>Superconductivity and possible variable range hopping in (TiZrNbCu)_{1-x}Ni_x, (TiZrNbNi)_{1-x}Cu_x and (TiZrNbCu)_{1-x}Co_x complex amorphous alloys</i> |
| P-3 | Liam Chandler, Liverpool <i>Multiscale quasiperiodic metallic alloys and characterising their physical properties</i> |
| P-4 | Natalia Glorizova, Dresden <i>From simple to complex structures one step at a time: calcium-containing nitridochromates</i> |
| P-5 | Bruno Gudac, Zagreb <i>Truly colossal negative magnetoresistance in EuCd₂As₂ at low temperatures</i> |
| P-6 | Büşra Mete, Dresden <i>Nb-Ni binary compounds in oxygen evolution reaction</i> |
| P-7 | Pavol Noga, Bratislava <i>High-fluence ion irradiation for materials testing</i> |
| P-8 | Gaurav Pransu, Zagreb <i>Photoresponse behavior of Dye Sensitized Solar Cells</i> |
| P-9 | Pavol Priputen, Bratislava <i>Characterization of Ga-Ni-Co-Cr-Fe-based multi-principal element alloys</i> |
| P-10 | Radoslaw Strzalka, Kraków <i>Phase transformation in decagonal Al-Cu-Rh quasicrystals induced by phasons</i> |
| P-11 | Yuki Utsumi Boucher, Zagreb <i>Emergence of intercalated transition metal derived bands near the Fermi level of (Co, Ni)_{1/3}NbS₂</i> |
| P-12 | Seyed Ashkan Moghadam Ziabari, Zagreb <i>Synthesis and characterization of magnetic transition metal chalcogenides</i> |
| P-13 | Ana Smontara, Zagreb <i>Contributions to the understanding of thermal and electronic transport in complex metallic compounds: from periodic to quasi-periodic crystals</i> |
| P-14 | Anton Kabaši, Split <i>Tuning thermal conductivity of hydrogen fuel cell catalyst films</i> |
| P-15 | Sylvain Le Tonquesse, Dresden <i>Influence of surface oxidation on the OER activity and stability of ZrNi and ZrCo</i> |

***Abstracts
of oral contributions***

Compositionally complex alloys: some problems and prospects

¹E. Babić*, ¹M. Basletić, ²I. A. Figueroa, ³M. Laurent-Brocq, ⁴S. Michalik, ⁵P. Pervan, ⁶R. Ristić, ⁷A. Salčinović-Fetić, ⁵D. Starešinić and ¹K. Zadro¹

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Despite a huge expansion of research on compositionally complex alloys, CCA (such as the entropy alloys, HEA and the corresponding glassy alloys) their comprehension is still limited, which is detrimental both for the design of CCAs and for their application. The broad compositional range in CCAs enables simple tuning of their properties by varying the contents of their constituent elements. Accordingly, the study of transition from CCA to conventional alloy, CA composed from the same constituents is important, both for understanding the formation of solid solutions in CCAs and for proper evaluation of their potential with respect to that of CAs. However, this transition has so far been studied systematically in only two types of alloys: isopleths of the Cantor alloy and glassy TiZrNbCuNi/Co alloys with variable Co, Ni or Cu content (Materials 14 (2021) 5824 and ref. therein). In both alloy systems the variation of a given property with composition depends sharply on the selected principal component and can be either monotonic (like that in the ideal solid solution) or non-monotonic. When the variation is non-monotonic, the maximum value of the selected property is usually outside of HEA composition range.

Emergence of long-range magnetic order from spin-glass state by tuning electron density in Ga-based 1/1 quasicrystal approximant

Farid Labib^{1*}, Shintaro Suzuki¹, Asuka Ishikawa², Takenori Fujii³ and Ryuji Tamura¹

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This study reports the first observation of ferromagnetic (FM) order in the non-Au-based approximant crystals (ACs) using a novel approach whereby a total electron-per-atom (e/a) ratio of the spin-glass Ga₅₀Pd₃₆Gd₁₄ 1/1 AC is lowered by simultaneously substituting certain ratios of a tri-valent Ga and a zero-valent Pd by a mono-valent Au. The emergence of FM order by this method was confirmed via magnetic susceptibility, magnetization, and specific heat measurements. The findings of this study open up vast opportunities in developing more long-range magnetic orders from ACs, quasicrystals, and even other RKKY compounds with spin-glass behavior.

Nodal-line driven anomalous susceptibility in ZrSiS

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We shall present a unique approach to test the signature of the nodal-line physics by thermodynamic methods. By measuring magnetic susceptibility in ZrSiS we found an intriguing temperature-driven crossover from dia- to paramagnetic behavior. We show that the anomalous behavior represents a real thermodynamic signature of the underlying nodal-line physics through the means of chemical pressure (isovalent substitution of Zr for Hf), quantum oscillations, and theoretical modeling. The anomalous part of the susceptibility is orbital by nature, and it arises due to the vicinity of the Fermi level to a degeneracy point created by the crossing of two nodal lines.

Furthermore, an unexpected Lifshitz topological transition at the degeneracy point is revealed by tuning the Fermi level. The present findings in ZrSiS give a new and attractive starting point for various nodal-line physics-related phenomena to be tested by thermodynamic methods in other related materials.

***Pressure evolution of electronic and crystal structures
of EuTGe_3 ($T = \text{Co, Rh, Ir}$)***

¹N. S. Dhami*, ²V. Balédent, ³O. Bednarchuk, ³D. Kaczorowski, ⁴S. R. Shieh, ⁵J. M. Ablett, ^{5,6}J.-P. Rueff, ⁵J. P. Itié, ¹C. M. N. Kumar, and ¹Y. Utsumi

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Intermetallic EuTX_3 (T: transition metal, X= Si/Ge) forms a non-centrosymmetric BaNiSn_3 -type structure and has been attracting considerable attention due to complex magnetic structures and unique pressure phase diagram that potentially accommodates superconductivity under pressure [1, 2]. At ambient pressure, EuTGe_3 series host divalent Eu ions ($4f^7$, $J=7/2$) and exhibit antiferromagnetic ordering at low temperature (< 15 K), while the ordering direction depends on the selection of T [1]. We studied the pressure evolution of the electronic and crystal structures of EuTGe_3 ($T = \text{Co, Rh, Ir}$) by high-resolution x-ray absorption spectroscopy and powder x-ray diffraction. Our study unveiled that the pressure gradient of the Eu valence change varies depending on T. By applying pressure, a continuous contraction of the lattice volume was observed in both EuCoGe_3 and EuRhGe_3 . EuIrGe_3 implied possible structural transition above 34 GPa.

This work is in part supported by the scientific project "Pressure- and Temperature-driven Phase transitions in Strongly Correlated Electron Systems (PaT PiSCES)"HrZZ UIP-2019-04-2154

References:

- [1] O. Bednarchuk et al., *J. Alloys Comp.* **622**, 432-439 (2015).
- [2] M. Nakashima et al., *J. Phys. Soc. Jpn.* **86**, 034708 (2017).

Growth of crystalline CoCrFeNi high-entropy alloy thin films by magnetron sputtering

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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). 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. We demonstrate the formation of crystalline thin films of CoCrFeNi via magnetron sputtering from homemade targets on MgO (100) and Al₂O₃ (0001) single crystal substrates. Following a proper UHV surface treatment, the structural and electronic behaviour is accessible by means of low energy electron diffraction and angle resolved photoelectron spectroscopy.

References:

- [1] Cantor et al., Mater. Sci. Eng. A, 213, **375-377**, (2004)
- [2] Yeh et al., Adv. Eng. Mater., 299-303, **6**, (2004)
- [3] Miracle et al., Acta Mater., 448, **122**, (2017)

Murunskite: a bridge between cuprates and pnictides

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Despite exceptional scientific efforts over several decades, there is almost no universal agreement about the superconducting state of cuprate compounds. A constructive way to improve understanding would be to synthesize and investigate a new system, which displays superior crystal chemical flexibility and tunability of the valence of the transition metal ions. One could then manipulate its various electronic, metallic, and mechanical properties. Here we study Murunskite, which interpolates between cuprates and pnictides[1]. In this presentation, I will present the successful growth and characterization of the first-ever high-quality Murunskite single crystals. These crystals show semiconducting behaviour in resistivity and optical transmittance, and antiferromagnetic ordering around 100 K. Spectroscopy (XPS) and Density Functional Theory (DFT) calculations concur that the sulfur 3*p* orbitals are partially open, making them accessible for charge manipulation, which is a prerequisite for superconductivity in analogous layered structures. Furthermore, DFT indicates that the valence band is more cuprate-like, while the conduction band is more pnictide-like. We also managed to electron-dope the parent compound, whose transport and optical conductivity measurements will be discussed in the presentation.

Reference:

[1] D.Tolj, et al, Applied Materials Today, Volume 24, 101096, (2021).

High throughput in-vivo toxicity test of organo-metallic photovoltaic perovskites via micro fluidics on the C. elegans

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The organo-metallic photovoltaic (PV) perovskite ($\text{CH}_3\text{NH}_3\text{PbI}_3$) has reached more than 25% conversion efficiency (in single junction configuration [1]), which suggests its imminent commercialization. Before public usage its health hazard needs to be addressed because of the lead in the formula. We have examined in-vivo toxicity of two types of PV perovskites; $\text{CH}_3\text{NH}_3\text{PbI}_3$ and its possibly less toxic sister compound $\text{CH}_3\text{NH}_3\text{SnI}_3$. Assessment was conducted on common model for soil toxicity, nematode *C. Elegans*. Novel high-throughput microfluidic platform was used, which frees toxicity experiments from tedious manual work and allows automated systematic approach. Main intoxication path and effect of perovskites on worms development and progeny was addressed, which is very important for design of health restrictions for this type of solar cells.

Reference:

- [1] "Best Research-Cell Efficiencies" National Renewable Energy Laboratory, June 30, 2022.

Collective plasmon modes of Dirac electrons in composite systems

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We study the coupling between plasmon modes due to the long-range Coulomb electron–electron interaction for a composite system consisting of a two-dimensional system of Dirac electrons placed in three-dimensional Dirac semimetal [1]. The mixing of the collective plasmon modes is obtained as the two-dimensional acoustic plasmon mode dispersion crosses the bulk plasmon mode. We show that the coupled plasmon modes become more separated with decreasing spacing between the two subsystems as the coupling increases due to the enhanced Coulomb interaction between electrons from different subsystems. We also investigate the effects of the Dirac cone tilts and anisotropies on coupled plasmon modes in both subsystems and find that they increase the coupled plasmon mode energies and renormalize their spectral weights [2]. The anisotropic effects of tilts are more significant for the larger separations of the subsystems when the Coulomb coupling is weaker.

References:

- [1] Ž. Bonačić Lošić, *Physica E* **120** (2020) 114094.
- [2] Ž. Bonačić Lošić, *Physica B* **615** (2021) 413124.

Thermal conductivity and lattice dynamics of aperiodic crystals

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The lattice thermal conductivity of many aperiodic crystals displays a ‘glass like behavior’ [1], with a relatively small value of the lattice thermal conductivity at ambient temperature and an almost independent temperature dependence in the range 20 to 300 K. The Umklapp peak observed in simple structure is largely suppressed. This is true for instance for the icosahedral quasicrystal i-AlPdMn [2], but also for the Rb₂ZnCl₄ phase that displays an incommensurately modulated phase between 190 and 300 K [3]. The detailed understanding of this behavior is still a matter of debate.

In this presentation we propose to apply a simple modified Debye model of a phonon lattice gaz, as developed for Ge based clathrates [4]. It is based on two assumptions: (i) the acoustic regime for which heat is carried by phonon is limited and characterized by a cut-off energy; (ii) higher energy excitations do not carry heat since they are almost dispersion less (see also [5]). Using this simple model it is possible to calculate an average phonon lifetime which will be compared to phonon measurements in different aperiodic crystals. Implication and contribution of phason modes will be also discussed [6].

References:

- [1] D. G. Cahill, S. K. Watson, and R. O. Pohl, *Physical Review B* **46**, 6131 (1992).
- [2] M. A. Chernikov, A. Bianchi, and H. R. Ott, *Physical Review B* **51**, 153 (1995).
- [3] D.-M. Zhu and A. C. Anderson, *J. Low Temp. Phys.* **94**, 117 (1994).
- [4] P.-F. Lory et al., *Nature Communications* **8**, 491 (2017).
- [5] T. Takeuchi, N. Nagasako, R. Asahi, and U. Mizutani, *Physical Review B* **74**, 054206 (2006).
- [6] T. Janssen, G. Chapuis, and M. de Boissieu, *Aperiodic Crystals. From modulated phases to quasicrystals (second edition)* (Oxford University Press, Oxford, 2018), Vol. 20, IUCr Monographs on Crystallography.

Electronic topology driven by strong correlations

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Complexity has many faces, one of them being strongly correlated ternary intermetallic compounds that are further enriched by nontrivial electronic topology. I will provide an overview of the recent activities of the Quantum Materials group at TU Wien in this emerging field. They range from investigations of the first Weyl-Kondo semimetal $\text{Ce}_3\text{Bi}_4\text{Pd}_3$ [1] and its relatives, to the exploration of topological phases and topological phase transitions by tuning [2], and the search for new topological phases by exploiting crystal symmetries [3] and quantum fluctuations [4].

References:

- [1] S. Dzsaber et al., PNAS **118**, e2013386118 (2021).
- [2] S. Dzsaber et al., Nat. Commun. **13**, 5729 (2022).
- [3] L. Chen et al., Nat. Phys. **913**, 191(2022).
- [4] W. T. Fuhrman et al., Sci. Adv. **7**, eabf9134 (2021); H. Hu et al., arXiv:2110.06182.

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Specific heat of topological semimetals and insulators across the correlation spectrum

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The past decade has seen a wealth of investigations on materials that are considered as topological semimetals and insulators. In the by far best studied regime of noninteracting or weakly interacting topological materials, key characterization tools are ARPES and quantum oscillation experiments together with density functional theory. In the recently evidenced strong correlation regime, by contrast, these tools fail and new ones have been put forward, with specific heat measurements being one of them [1-4].

In this presentation we report a systematic study of low-temperature specific heat in topological materials across the correlation spectrum. We will discuss which information specific heat can provide in the weakly interacting regime. The ground states of these materials are discussed, taking also recent studies of their charge transport properties, ARPES, and density functional theory calculations into account.

References:

- [1] L. Chen et al., Nat. Phys. (2022). DOI:10.1038/s41567-022-01743-4
- [2] S. Dzsaber et al., Nat. Commun. **13**:5729 (2022).
- [3] S. Dzsaber et al., Proc. Natl. Acad. Sci.U.S.A. **118**, e2013386118 (2021).
- [4] M. Taupin et al., arXiv:2010.10620v1 (2020).

Electrical transport in half-Heusler compound TmPdSb

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In recent years, rare-earth-based half-Heusler (HH) pnictides have gained tremendous attention due to a range of non-trivial physical properties that have opened the door to various applications, such as in spintronics, green energy harvesting or quantum computing. Although many HH phases have been investigated in depth, some are still poorly characterized.

In this work, we studied the structural, magnetic, and electrical transport properties of TmPdSb single crystals, synthesized from Bi flux. The compound was found to have a MgAgAs-type structure, typical for HH materials, and to exhibit a Curie-Weiss paramagnetism down to 2 K due to the magnetic moments carried on Tm³⁺ ions. Its electrical conductivity, measured along the [001] direction, shows a semiconducting character at high temperatures and a metallic behavior below about 50 K. This finding is consistent with the variation in carrier (electron) concentration, derived from the Hall effect data. Below 10 K, the magnetic field-dependent conductivity in TmPdSb is governed by a weak antilocalization effect.

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Anomalous electrical transport in EuZn₂Sb₂

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Manipulation of charge transport by spin degrees of freedom has attracted a great interest in topological materials because of their exotic fundamental physics and potential applications. In this context, the compounds EuCd₂As₂ and EuZn₂As₂ gained special attention [1,2].

In this work, we studied the structural, thermodynamic and electrical transport properties of high-quality single crystals of EuZn₂Sb₂. Alike the arsenides, the compound has a trigonal CaAl₂Si₂-type crystal structure, and orders antiferromagnetically (AFM) at low temperatures due to Eu²⁺ ions. The AFM structure is A type with the magnetic moments confined in the hexagonal *ab* plane. In external in-plane magnetic field, a spin flop transition occurs. Most interestingly, in the canted AFM state, the transverse magnetoresistance shows a distinct hump and the Hall resistivity becomes highly non-linear. These unusual transport features likely arise due to the non-collinear spin structure with finite vector spin chirality.

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

References:

- [1] J.-R. Soh, et al., Phys. Rev. B 100, 201102(R) (2019).
- [2] Z.-C. Wang, et. al., Phys. Rev. B 105, 165122 (2022).

Complexities of 2H-NbS₂ intercalations

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2H-NbS₂ is superconducting, quasi 2D system, which can host different ions and molecules in van der Waals gaps between metallic layers. When intercalated with transition metal (TM) ions system becomes magnetic. The coexistence of metallic and magnetic degrees of freedom coupled with reduced dimensionality and anticipated frustration renders these compounds battlefield of different interactions resulting in different magnetically ordered ground states.

We have studied Ni and Co [1,2,3] intercalations. The degree of crystal order plays a vital role in obtaining correct conclusions. Thus, we started with synthesis and detailed characterization and managed to correlate physical properties with structural complexities. Finally, using angle-resolved photoelectron spectroscopy (ARPES), we identified limitations of the DFT calculations casting new light on these compounds.

This work is in part supported by the scientific project „Intercalated transition metal dichalcogenides“ (HrZZ IP-2020-02-9666).

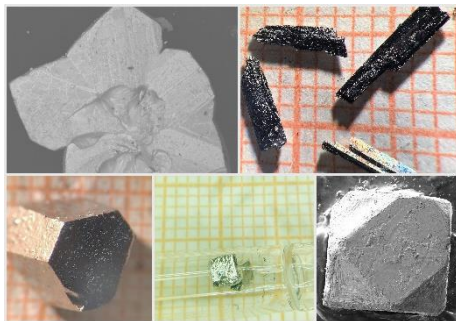
References:

- [1] N. Barišić et al. Phys. Rev. B, **84** (2011) 075157.
- [2] P. Popčević et al. arXiv: 2003.08127.
- [3] P. Popčević, Y. Utsumi et al. Phys. Rev. B, 105 (2022) 155114.

Superconductivity and magnetism in complex mercury-based compounds^{1,*}E. Svanidze, ¹Yu. Prots, ¹Yu. Grin¹Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Strasse 40,
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Mercury, in both elemental form and as part of compounds and amalgams has played an important role in solid-state chemistry and condensed matter physics [1-3]. However, much care must be taken both during synthesis as well as during characterization of this peculiar element and its compounds – from toxicity concerns to high chemical reactivity – these systems pose several experimental challenges. In this talk, I will showcase that, nonetheless, mercury-based materials offer unique crystallographic motifs and, as a result, peculiar physical properties [4-6]. In particular, I will concentrate on the binary compounds of mercury and lanthanide as well as



actinide elements, which have so far been under investigated. Using a unique laboratory environment, we are able to synthesize single crystals of several binary phases (Figure 1) and study their chemical and physical properties in detail. By looking at the evolution of crystallographic complexity across several series of compounds, I will discuss how intrinsic crystal chemistry affects the resultant ground states.

Figure 1: Examples of single crystals of mercury-based materials.

References:

- [1] F. Tambornino and C. Hoch, *Zeitschrift Anorg. Allg. Chemie* **641**, 537 (2015).
- [2] C. Hoch and A. Simon, *Angew. Chemie Int. Ed.* **51**, 3262 (2012).
- [3] F. Merlo and M. L. Fornasini, *J. Less-Common Met.* **64**, 221 (1979).
- [4] E. Svanidze, A. Amon, R. Borth, Y. Prots, M. Schmidt, M. Nicklas, A. Leithe-Jasper, and Y. Grin, *Phys. Rev. B* **99**, 220403 (2019).
- [5] Y. Prots, M. Krnel, Y. Grin, and E. Svanidze, *Inorg. Chem.* **61**, 39, 15444 (2022).
- [6] Y. Prots, M. Krnel, M. Schmidt, Y. Grin, and E. Svanidze, *Phys. Rev. B* **106**, L060412 (2022)

Superconductivity in crystallographically disordered LaHg_{6.4}

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Although typically, the lack of translational symmetry prohibits the appearance of superconductivity, the coexistence of the latter with structural disorder has been observed in some materials [1-3]. However the influence of structural disorder on superconductivity is not yet fully understood. Hg-based materials often have complex crystallographic arrangements making them candidates for interesting physical properties. A detailed examination of crystallographic and physical properties of LaHg_{6.4} [4] reveals that this material has a transition to a superconducting state at $T_c = 2.4$ K while showing crystallographic disorder in one dimension. We were able to determine in detail the structure type of Lanthanum mercuride (space group Cmc₂m, $a = 9.779(2)$ Å, $b = 28.891(4)$ Å, $c = 5.0012(8)$ Å, $Z = 8$), which has remained out of reach for nearly 50 years. In this crystal structure, strong disorder is present in the channels that propagate along the [001] direction. By using a combination of specific synthesis and characterization techniques, we were able to avoid the problems associated with the low formation temperature and chemical reactivity of this substance, thus making it possible to study the physical properties of LaHg_{6.4}.

References:

- [1] C. Brun *et al.*, Nat. Phys. **2014**, 10, 444–450.
- [2] J. Peng *et al.*, ACS Nano **2018**, 12, 9461–9466.
- [3] H. Ji *et al.*, Adv. Phys. X **2021**, 6, 1884133.
- [4] Y. Prots *et al.*, Inorg. Chem. **2022**, 61(39), 15444–15451.

***Effects of hydrostatic pressure on the Weyl-Kondo semimetal candidate
CeRu₄Sn₆***

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The interplay of nontrivial electronic topology and strong correlations can lead to the realization of entirely new quantum phases, and thus is of great current interest. A prime example is the newly discovered Weyl-Kondo semimetal phase realized in Ce₃Bi₄Pd₃ [1-3]. There, a cubic-in-temperature contribution to the electronic specific heat [1] and a giant spontaneous Hall response [3] are attributed to the presence of Weyl nodes in the immediate vicinity of the Fermi energy. Another candidate material theoretically predicted to host Weyl points near E_F is the tetragonal, noncentrosymmetric Kondo semimetal CeRu₄Sn₆ [4]. The recent discovery that CeRu₄Sn₆ is quantum critical without tuning [5], makes it a unique platform to study the possible role of quantum criticality in the formation mechanism of Weyl-Kondo semimetals. Here we probe the phase diagram of CeRu₄Sn₆ by means of electrical transport and specific heat measurements under hydrostatic pressure and discuss evidence for Weyl-Kondo physics emerging at finite pressure.

References:

- [1] S. Dzsaber et al., Phys. Rev. Lett., **118**, 246601 (2017)
- [2] H.-H. Lai et al., Proc. Natl. Acad. Sci. U.S.A. **115**, 93 (2018)
- [3] S. Dzsaber et al., Proc. Natl. Acad. Sci. U.S.A. **118**, e2013386118 (2021)
- [4] Y. Xu et al., Phys. Rev. X **7**, 011027 (2017)
- [5] W. T. Fuhrman et al., Sci. Adv. **7**, eabf9134 (2021)

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Chemical bonding and structural complexity

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A common strategy to describe CMA from a geometric point of view is the grouping of atoms into local atomic arrangements (crystallographic clusters), which makes the crystal structure easier to visualize, to perceive and understand the geometric organisation; it reduces the degree of complexity and allows to relate the CMA to simpler crystal structures. This is the nested-polyhedra units approach, which was introduced first for the description of the γ -brass-derived structures. The choice of a crystallographic cluster is considered as reasonable, if its shells are as spherical as possible and are quite separate with respect to the distances between the shells and with respect to the centre of the nested polyhedrons. On the other hand, the so defined crystallographic clusters are not in agreement with the chemical definition of such an entity, as the chemical definition entails atomic interactions within the chemical clusters that are stronger than the interaction of the clusters with neighbouring aggregates, would be preferable, thus raising the question about the stabilization mechanisms for these structural. Quantum chemical investigations of chemical bonding in CMA are naturally hindered by the huge size of the unit cells and inherent disorder. In particular, the role of the charge transfer in the stabilization was studied on example of the CMA $\text{Mg}_{29-x}\text{Pt}_{4+y}$ [1] in comparison with $\text{Be}_{21}\text{Pt}_5$ [2], and their chemically analogous but non-complex Be_5Pt [3].

References:

- [1] L. Agnarelli et al. Inorg. Chem. (2022) in print.
- [2] A. Amon et al. Acc. Chem. Res. 51 (2018) 214.
- [3] A. Amon et al. Angew. Chem. Int. Edit. 58 (2019) 2.

***Catalytic and material complexity –
In-Pt/In₂O₃ in methanol steam reforming***

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Changing our energy supply towards a renewable and sustainable energy scenario requires storage and transport of large amounts of renewable energy. Due to their high chemical storage capacity for hydrogen, small molecules like CH₄, NH₃ or methanol are promising candidates. Methanol is liquid at normal conditions and possesses a high volumetric and gravimetric energy density.^[1] To release the hydrogen on demand, methanol steam reforming can be applied (CH₃OH + H₂O → 3 H₂ + CO₂). Since the identification of ZnPd/ZnO as highly selective catalyst^[2], it could be shown that high selectivity is achieved only if ZnPd and ZnO are present^[3]. While the necessity could be shown, it is still unclear how the phases contribute to the catalytic cycle.

Recent material development led to the discovery of the very active and selective aerogel-based material In-Pt/ In₂O₃^[4]. To clarify active phases, the oxide-metal interplay and the role of the oxidic species in the catalysis numerous in situ and operando methods as well as isotope-labelling of the reactants was conducted. This resulted in the detection of a Mars-van-Krevelen mechanism, the involvement of oxygen vacancies in the catalytic cycle as well as a delicate interplay between the oxygen potential of the atmosphere and the phases present in the catalyst. In addition, the underlying reason for deactivation of the materials could be revealed, opening the possibility for further development of materials, thus contributing to the energy turnaround.

References:

- [1] F. Asinger, Methanol – Chemie- und Energierohstoff, Springer, Berlin and Heidelberg, **1986**.
- [2] N. Iwasa et al. Catal. Lett. **1998**, 54, 119.
- [3] M. Friedrich et al. J. Catal. **2012**, 285, 41.
- [4] N. Köwitsch et al. J. Phys. Chem. C **2021**, 125, 9809.

Size-dependent methanol steam reforming investigated on unsupported ZnPd nanoparticles

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ZnPd-based catalysts for methanol steam reforming (MSR) have superior stability without being pyrophoric and possess comparable CO₂ selectivity (about 99%) to commercial Cu-based catalysts[1-3]. As of now, supported ZnPd/ZnO systems have addressed the impact of ZnPd-particle size on the catalytic characteristics in MSR. However, no conclusive evidence was obtained regarding how the particle size affects the catalytic properties of ZnPd/ZnO in MSR[2,4,5]. To simplify the materials, unsupported ZnPd with different crystallite sizes have been successfully synthesized via electroless plating without the use of surfactants. These materials enable to address the size influence on the catalytic properties in methanol steam reforming without the influence of the supporting ZnO. Characterization after catalysis revealed that the smaller starting particles showed more severe sintering which turned the sample into the larger sized particles, which might be the reason for the inconclusive results described in literature.

References:

- [1] M. Armbrüster et al., *Catal. Rev.: Sci. Eng.* 55, 2013, 289.
- [2] A. Karim et al., *J. Catal.* 243 (2), 2006, 420.
- [3] J. Shen et al., *Catal. Today*, 77 81-2, 2002, 89.
- [4] R. A. Dagle et al., *Top. Catal.*, 46 (3-4), 2007, 358.
- [5] K. Lim et al., *J. Phy. Chem. B*, 110 (30) 2006, 14890.

**Chemical behaviour of Mo_2TMB_2 (TM: Fe, Co, Ni)
upon oxygen evolution reaction (OER)**

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Oxygen evolution reaction (OER) is the slowest step of water electrolysis, demanding an active electrocatalyst, that should be also stable under strong oxidative conditions of OER. With the help of (partially) ordered crystal structures and well-defined electronic states of the elements in these compounds, intermetallic compounds possess an interesting class of materials for electrocatalysis. ^[1] The binary compounds in Mo-Ni and Mo-B systems were extensively studied as electrocatalysts for the hydrogen evolution reaction (HER). ^[2-4] In present study, intermetallic compounds Mo_2TMB_2 (TM: Fe, Co, Ni) were extensively investigated under conditions of OER in alkaline media.

While Mo_2CoB_2 and Mo_2NiB_2 crystallizes with W_2CoB_2 structure type (Immm, $a = 7.087(2) \text{ \AA}$, $b = 4.584(3) \text{ \AA}$, $c = 3.164(5) \text{ \AA}$ for Mo_2CoB_2 and $a = 7.075(5) \text{ \AA}$, $b = 4.557(5) \text{ \AA}$, $c = 3.179(5) \text{ \AA}$ for Mo_2NiB_2), Mo_2FeB_2 possesses U_3Si_2 -type of structure (P4/mbm, $a = 5.807(4) \text{ \AA}$, $c = 3.142(3) \text{ \AA}$). These compounds were synthesized via arc melting of initial materials, followed by homogenization annealing and manufacturing of the electrodes using spark plasma sintering (SPS). Chemical behaviour of Mo_2TMB_2 under OER conditions was studied using electrochemical techniques as well as comprehensive characterization methods.

References:

- [1] L. Rößner, M. Armbrüster, ACS Catal. 9, 2018 (2019).
- [2] J.M. Jakšić, M.V. Vojnović, N.V. Krstajić, Electrochim. Acta 45, 4151 (2000).
- [3] L. Rößner, H. Schwarz, I. Veremchuk, et al., ACS Appl. Mater. Interfaces, 13, 23616 (2021).
- [4] H. Park, A. Encinas, J. P. Scheifers, et al., Angew. Chem. Int. Ed. 56, 5575 (2017).

Surface properties of Ga₃Ni₂ and In₃Ni₂ intermetallic catalysts

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We present the recent studies of surface structures and chemical properties of Ga₃Ni₂ and In₃Ni₂ intermetallic catalysts by various surface science techniques, namely, x-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM).

XPS reveals that all three high symmetry surfaces; (100), (001), and (2-10); of Ga₃Ni₂ prepared by the usual method of sputtering and annealing demonstrate segregation of Ga to the surface. However, the surfaces are still highly ordered as revealed by LEED and STM. The Ga₃Ni₂(100) and Ga₃Ni₂(010) surfaces are bulk truncated, while the Ga₃Ni₂(2-10) surface shows a c-(2×2) reconstruction. Exposure of O₂ to the Ga₃Ni₂(001) surface selectively oxidises Ga but Ni core levels are not affected.

The In₃Ni₂(100) and In₃Ni₂(001) surfaces are also bulk truncated but the In₃Ni₂(2-10) surface demonstrates a (2×1) reconstruction. The In₃Ni₂(001) surface yields a c-(2√3×4) rectangular superstructure with three domains upon exposure to H₂. The superstructure is removed and the (1×1) structure is recovered after annealing the surface.

Structural stability of In-Pd intermetallic nanoalloys¹A. Front, ¹C. Lapointe, ¹E. Gaudry¹UL-CNRS, Institut Jean Lamour, UMR7198, Nancy, France

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At the nanoscale, materials exhibit unique properties that differ greatly from those of the bulk state. In this context, atomic arrangements of nanoalloys must be perfectly characterized in order to master and tune physical-chemistry properties. Transition metal based nanoalloys have been extensively investigated both experimentally and theoretically [1]. However the search of sustainable materials imposes to go beyond. Intermetallic nanoalloys may be a key. In-Pd nanoalloys have been synthesized mainly for their unique catalytic properties [2-3]. The main bottleneck in the development of intermetallic nanoalloys is the lack of structural characterization.

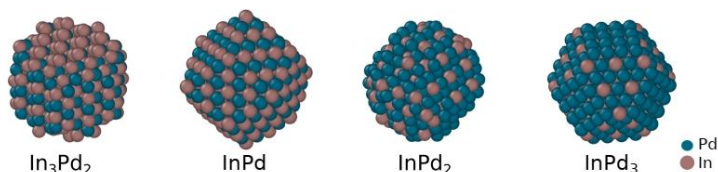


Fig. 1: Stable structures of ordered intermetallic In-Pd nanoalloys designed with a radius of 25 Ång. within a Wulff shape.

We have adopted a multiscale approach using DFT calculations and atomistic modelling to investigate structural stability as a function of sizes and compositions of In-Pd nanoalloys. Equilibrium crystalline shapes have been determined with the Wulff theorem and compare to other structures. The most stable nanoparticles are those chemically ordered showing a Wulff shape (Fig. 1). Disordered nanoparticles are less stable and become amorphous when the concentration of In increases.

References:

- [1] R. Ferrando *et al*, *Chem. Rev.* 2008, 108, 3, 845-910
- [2] N. Köwitsch *et al*, *ACS catalysis* 2021, 11, 1, 304-312
- [3] A. Garcia-Trenco *et al*, *Applied Catalysis B:Environmental* 2018, 220

**Complex ultrathin oxide structures revealed by
evolutionary computations : $\text{In}_x\text{O}_y/\text{PdIn}(001)$**

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The formation of complex oxide structures is possible when two-dimensional (2D) oxide materials are grown on intermetallic single crystal substrates [1]. Modelling such phases using Density Functional Theory (DFT) computations is a challenging task. It has been shown for recently discovered ultrathin quasicrystal structures that methods of tiling, using particular atomic decorations for the tiles, can be used to develop such models [2]. Crystal structures of two-dimensional materials may also be predicted with great accuracy by evolutionary algorithms [3]. In this work, we concentrate on ultrathin complex indium oxide films produced on a PdIn(001) single crystal substrate. The atomic structures of these ultrathin oxide films are determined using a combination of DFT and evolutionary calculations. In the end, 114 models are chosen based on their formation energies, displaying a (1×3) , (1×5) , or (1×7) supercell. Their stability is examined using surface energy calculations with two thermodynamic models to take into consideration the growing conditions and electronic structure calculations. In conclusion, based on evolutionary simulations, this work reveals plausible configurations for ultrathin oxide films produced on PdIn(001), generating a database with all structural and electronic information for the best structures, which will serve as a valuable road map for future experimental evaluation.

References:

- [1] Forster et al., *Phys. Rev. Lett.* 117 (2016) 095501
- [2] C. Merchan et al., *Phys. Chem. Chem. Phys.*, 24 (2022) 7253
- [3] F. Brix and E. Gaudry, *Journal of Vacuum Science & Technology A* 40 (2022) 012203

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Surface composition & oxidation studies of Ga₃Ni₂ intermetallic alloy catalyst

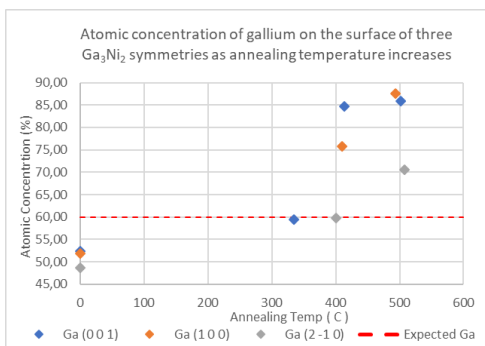
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Ga₃Ni₂ has been reported as a potential heterogeneous catalyst in the hydrogenation of CO into methanol at atmospheric pressure [1]. Understanding the surface of a catalyst is paramount to get insight to the chemical processes [2].

To understand the optimal surface preparation conditions, X-ray photoelectron spectroscopy (XPS) is used to monitor the changes in the surface composition after sputtering and annealing at different temperatures from 250°C – 510°C. All high symmetry surfaces (100), (001) and (2-10) were studied by XPS.



For all three surfaces sputtering preferentially removed gallium, the heavier of the two elements, from the sample. After annealing the surface to temperatures >400°C gallium segregates from the bulk to the surface. The segregation was observed by XPS as an increase in the percentage of gallium on the surface from the expected 60% gallium to a maximum of 87.6%.

Angular resolved XPS from the surfaces confirms that the increase in gallium atomic concentration observed is on the top layers of all three surfaces. Despite this gallium segregation on the surface, surfaces are highly ordered as clear LEED patterns were observed and STM also shows large flat terraces with atomic resolution.

After exposing the Ga₃Ni₂ (0 0 1) surface to over 1000 Langmuir of oxygen, XPS showed that the Ga core levels have shifted to a higher binding energy. This confirms the presence of a gallium oxide. However, the nickel peaks remain unchanged in core level energy and shape for any exposure up to 1000 Langmuir.

- [1] Wencka, M., Kovač, J., Dasireddy, V.D., Likozar, B., Jelen, A., Vrtnik, S., Gille, P., Kim, H.J. and Dolinšek, J., 2018. *Journal of Analytical Science and Technology*, 9(1), pp.1-10
- [2] Urban, K., 2010. *Complex metallic alloys: fundamentals and applications*. John Wiley & Sons.

Coherent interface between diamond and clathrate structures

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Diamond and clathrate structures can form coherent, sp³-bonded interface stable against annealing at temperatures approaching melting point of the constituents, and bearing over 15% tensile deformation in ab-initio model simulations. Bonding between the two structures occurs via common transitional layer known as 3×3 dimer-stacking fault (DS) reconstruction on the diamond side, matching a layer with identical geometry found in clathrate type II or III. The uniform-chemistry interface ~10% mismatch can be eliminated by tuning composition of one or both constituent structures. Appropriate diamond-structure support can be used to grow new metastable clathrate compositions.

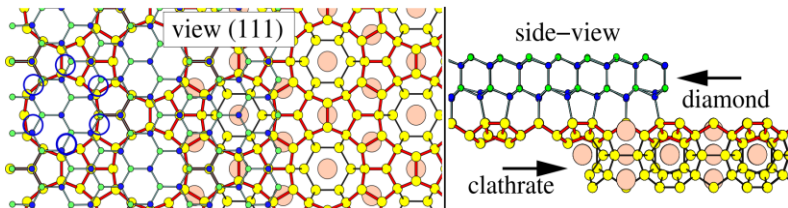


Figure: diamond/clathrate InN/NaSi interface. In atoms are shown blue, N green, clathrate Si yellow and Na pink-orange.

Revealing the epitaxial interface between $Al_{13}Fe_4$ and Al_5Fe_2

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Interfaces are known to play an important role in a broad range of scientific and technological fields. Their design is crucial to improve the performances of heterostructures. In metallurgy, aluminized steel combines the low weight of aluminium with the high strength of steel. But the distinct thermal and physical properties of Al and Fe metals make it challenging to join. Buffer layers made of Al-Fe intermetallic compounds generally forms at the interface. Their nature depends on the chemical potentials, the nucleation conditions and the mobilities of the elements.

On the basis of surface X-ray diffraction (SXRD), combined with calculations based on Density Functional Theory (DFT), we derive in this work a consistent model at the atomic scale for the complex $Fe_4Al_{13} // Fe_2Al_5$ interface (Fig. 1). Calculations of adhesion and constrain energies for several structural models identify the lattice mismatch and the composition of the interfacial plane as a main factor for the stability. The matching of the [001] direction of Fe_2Al_5 with the [010] direction of Fe_4Al_{13} supports a mechanism of easy Al diffusion in the Al-Fe system, to explain the formation of the complex Fe_4Al_{13} and Fe_2Al_5 phases at the interface.

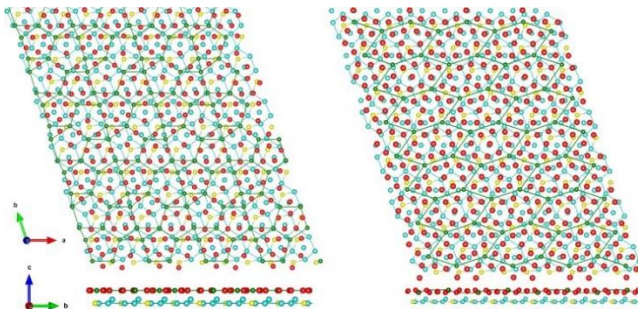


Fig 1: Structure of the Giant interfacial model. The Al_5Fe_2 phase is depicted by cyan (Al) yellow (Fe), $Al_{13}Fe_4$ phase using red (Al) and green (Fe) spheres.

Structural investigation of the Ho-Au-Si (100) approximant surface

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RE-Au-Si (RE=Gd,Tb,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 RE atom leading to alteration of magnetic and thermoelectric properties[1].

Unlike for the bulk, the surface atomic structure and properties of RE-Au-Si systems remain unexplored. Several key questions are awaiting answers including the influence of the cluster center decoration on the surface plane selection and on the structural stability of surface layers.

To this end, we report the characterization of the (100) surface of the $\text{Ho}_{1.04}\text{Au}_{4.85}\text{Si}_{1.324}$ Tsai-type 1/1 approximant using both experimental techniques and Density Functional Theory (DFT)-based methods. Low energy electron diffraction (LEED) pattern, and high-resolution scanning tunneling microscopy (STM) images show a (2x1) surface reconstruction and selection of a specific bulk plane as surface layer. To determine the latter, DFT calculations have been performed on several surface models. Finally, the calculated bulk density of states dominated by Au 5d states show great similarities with ultra-violet photoelectron spectroscopy measurements.

Reference:

[1] G.H. Gebresenbut et al., J. Phys.: Condens. Matter 26, (2014) 322202.

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

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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 Ni₂MnGa 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. 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 (623K) [2]. We use scanning tunneling microscopy (STM) imaging and low-energy electron diffraction (LEED) to study the structural and microstructural changes occurring across the phase transition between the high temperature austenite with L2₁ structure and the low temperature martensite with seven-fold modulated monoclinic structure (Fig.1).

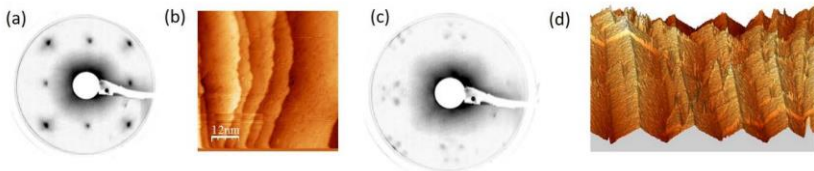


Fig. 1: LEED patterns and STM images of the austenite (a,b) and the martensite (c,d) phases.

References:

- [1] A.A. Cherechukin et al., Phys. Lett. A 291 (2001) 175
- [2] M. Takhsha Ghahfarokhi *et al.*, Acta Mat. 187 (2020) 135

Entropy engineering in materials for conversion energy (thermoelectrics & ion batteries)

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The efficiency of materials converting various forms of energy due to thermoelectric or electrochemical effects is partly related to peculiar electronic properties driving transport and electrochemical behaviors. The KKR-CPA method is implemented for electronic structure calculations to account for disorder in thermoelectric and ion-battery systems. The ab initio results combined with modeling of electron transport and electrochemical properties in selected thermoelectrics [1,2] and Li-/Na-ion batteries [3] are presented. Noteworthy, unusual electronic structure features appearing in these materials, namely band convergence, entropy induced band engineering (thermoelectrics) and specific character of charge/discharge curves correlated with electromotive force (batteries), directly determining their performance. Finally, recent studies of high-entropy oxides for the Na-ion cathode is discussed [4].

References:

- [1] B. Wiendlocha et al., Scripta Mater. 111 (2016) 33
- [2] O. Cherniushok et al. ACS Appl. Mater. Interfaces 13 (2021) 39606.
- [3] J. Molenda et al., Phys. Stat. Sol. A 217 (2020) 1900951.
- [4] K. Walczak et al., Energy Storage Mater. 47 (2022) 500

Size matters: a study on transport properties of type-I clathrate nanowires

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Sustainable solutions to our energy crisis are needed more urgently than ever. While not being the answer to all of our problems, thermoelectric materials play an important role in regaining some of the otherwise lost waste heat. Their conversion efficiency is defined by the dimensionless figure of merit $ZT = \sigma S^2 T / \kappa$, with the electrical conductivity σ , the thermopower S , the temperature T and the thermal conductivity κ . Therefore, a good thermoelectric material should have a high σ and S , but also a low κ . Here we present a size study on type-I clathrates, in which the phonon Kondo effect is held responsible for a flattening of the acoustic phonon modes in a sizable range of momentum space, thereby lowering the phonon thermal conductivity [1]. To scrutinize this picture, we use well-studied single crystals [2, 3] and shape them into nanowires with different diameters using a focused ion beam (FIB) technique. Because in the above picture only long-wavelength phonons carry heat in these materials, the dependence of κ on the diameter should be noticeable. Additionally, we compare the electrical resistivities of the nanowires to get a full picture of how size affects the transport properties of type-I clathrate nanowires.

References:

- [1] Ikeda, M.S. et al., Nat. Commun. **10**, 887 (2019)
- [2] Prokofiev, A. et al., Nat. Mater. **12**, 1096–1101 (2013)
- [3] Zhang, H. et al., Inorg. Chem. **50**, 1250–1257 (2011)

Structural complexity in the apparently simple crystal structure of Be₂Ru

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During the study of the Be-Ru binary system, the crystal structure of Be₂Ru was reinvestigated. Differently from what is reported in literature, Be₂Ru crystallizes with hexagonal Fe₂P-type structure. The crystal structure can be described as constituted by a substructure of ruthenium atoms arranged within planar layers in the form of condensed six-membered rings in the ab plane. The latter are separated by a layer formed by Be atoms found at half of the c axis' length of the unit cell, in a ABAB sequence. Analysis of the collected single-crystal data revealed a crystal structure more complicated than expected. In fact, an additional position very close in distance to the Ru1 atom can be recognised. The possibility of a stacking fault in the ab plane was advanced and a TEM investigation was carried out, which confirmed such hypothesis. The calculated electronic density of states (DOS), revealed that, contrary to typical intermetallic compounds, Be₂Ru shows a pseudo gap in the vicinity of the Fermi level. The temperature dependence of the electrical resistivity of Be₂Ru, shows metallic behaviour in agreement with the non-zero DOS at the Fermi level.

***Abstracts
of poster contributions***



Surface structure of In₃Ni₂ Inter-metallic compound

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Inter-metallic 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]. In₃Ni₂ acts as catalyst for hydrogenation of carbon dioxide into methanol [2]. Understanding of surface structure and electronic properties of In₃Ni₂ would help to learn and optimise the catalytical activities.

This work describes the first study of atomic structure of In₃Ni₂ by two surface science techniques, Scanning Tunnelling Microscopy (STM) and Low Energy Electron Diffraction (LEED). All high symmetry surfaces (100), (001) and (2⁻10) prepared by sputtering (Ar⁺ for 30 minutes, drain current 5-6 μA) and annealing at 350-550 °C.

We found that surface ordering starts at annealing temperature of 350 °C and high-quality LEED patterns are observed at 480 °C.

LEED patterns for two surfaces (100) and (001) reveal bulk truncated surface, (1x1) structure. However, surface (2⁻10) has (2x1) structure. Atomic resolution is obtained in STM images, which can be explained using the model atomic structure. Furthermore, the (001) surface shows a c-(2√3 x 4) rectangular superstructure with three domains that formed from deposit H₂-deposition, which is confirmed by both LEED and STM.

References:

- [1] M. Ivanov, V. Berezutskii, M. Shevchenko, V. Kudin, and V. Sudavtsova, Powder Metallurgy and Metal Ceramics, vol. 54, no. 7, pp. 465–470, 2015.
- [2] C. Li, Y. Chen, S. Zhang, S. Xu, J. Zhou, F. Wang, M. Wei, D. G. Evans, and X. Duan, Chemistry of Materials, vol. 25, no. 19, pp. 3888–3896, 2013.

P-2

Superconductivity and possible variable range hopping in (TiZrNbCu)_{(1-x)Ni_x}, (TiZrNbNi)_{(1-x)Cu_x} and (TiZrNbCu)_{(1-x)Co_x} complex amorphous alloys

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We present the result of a systematic study of electrical resistivity, superconductive transitions and Hall effect for three systems of compositionally complex amorphous alloys of early (TE) and late (TL) transition metals in a broad composition range x (0.1-0.5). All samples showed a high resistivity at room temperature (140-240 $\mu\Omega$ cm) and the superconducting transition temperatures decrease with increasing TL content, similar to binary amorphous [3] and crystalline HEA TE-TL alloys [4]. With the highest recorded transition for (TiZrNbCu)_{0.90}Co_{0.10} at 1.94 K. The Hall coefficient R_H is temperature independent and positive for all samples except for (TiZrNbCu)_{0.57}Co_{0.43} with an interpolated critical concentration at $x_c=0.34$, in good agreement with binary TE-TL alloys [1]. For the temperature dependence of resistivity, we discuss possible variable range hopping (VRH) like parallel conduction mode, in temperature range 30-150K, with an exponent $p=1/2$. We examine this in the context of VRH in granular materials [2].

References:

- [1] J. Ivkov and E. Babić, J. Phys.: Condens. Matter **2** (1990) 3891
- [2] V. F. Gantmakher, Electrons and Disorder in Solids (OUP Oxford, 2005).
- [3] E. Babić et al, Solid State Commun. **39** (1981) 139
- [4] K. Stolze et al, Chem. Mater. **30** (2018) 906



Multiscale quasiperiodic metallic alloys and characterising their physical properties

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Quasicrystals (QC) are complex metallic alloys with long-range crystallographic order and aperiodicity, leading to a unique combination of properties [1]. The structure of most common QCs has been understood and various novel structures have been observed in thin films on QC surfaces [2,3]. Quasiperiodic tilings are models which describe the atomic surface structure of QC; molecular overlayers have been shown to selectively adsorb on QC surfaces forming such tilings [2]. However, characterising the physical properties of these atomic-scale QC structures is challenging due to various limitations associated with UHV experiments.

The presenting research overcomes limitations by fabricating mesoscopic 2D quasiperiodic tilings of metallic alloys with thermal nanolithography. The aim of fabricating tilings with nanolithography is to understand the magnetic properties of tilings, in relation to QC structure. Ammann-Beenker, Penrose, and Fibonacci tilings have been fabricated, among others, with magnetic Ni₄Fe decorating the tilings and imaged with electron microscopy. These tilings model the surface of 8-fold, 5-fold, and 2-fold complex metallic alloys. In future, the tilings will be imaged with magnetic microscopy methods.

References:

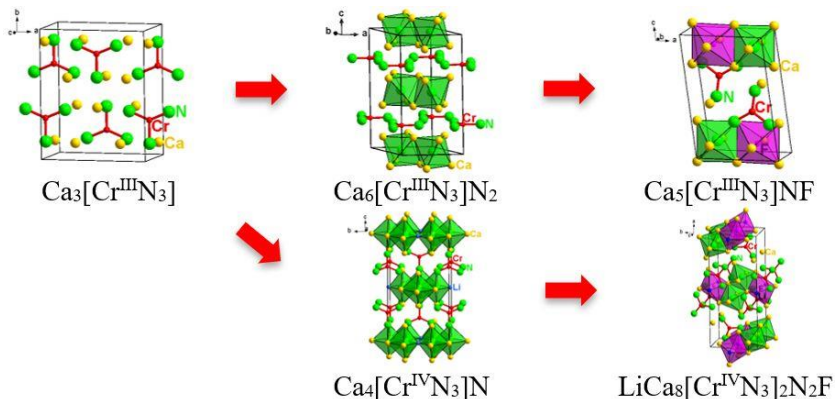
- [1] D. Shechtman and I. A. Blech. Metallurgical Transactions A, vol. 16, no. 6, pp. 1005–1012, 1985.
- [2] S. Coates, et al. Nature communications, vol. 9, no. 1, pp.1–5, 2018.
- [3] V. Fournée, et al. Recent Advances in Thin Films, pp. 13–34, Springer, 2020

P-4

From simple to complex structures one step at a time: calcium-containing nitridochromates^{1,*}N. Glorizova, ¹Yu. Prots, ¹Yu. Grin, ¹P. Höhn¹Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer str. 40, 01187, Dresden, Germany

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Exploratory research on calcium-containing nitridochromates with incorporation of lithium and fluoride resulted in a plethora of new compounds, crystallizing in often unique crystal structures. The complexity of the structures increases from simple 3:1:3 composition in $\text{Ca}_3[\text{Cr}^{\text{III}}\text{N}_3]$ ^[1] to nitridochromates with mixed anions, as well as cations. Different cationic and anionic species influenced the oxidation state of chromium and resulted in phases with Cr(III) and the otherwise mostly elusive Cr(IV). The compounds will be discussed with regards to corresponding prototype structures, as well as other known nitridochromates.

**Reference:**

- [1] Höhn, P. and R. Niewa, *Handbook of Solid State Chemistry*. 2017, Wiley-VCH. p. 251-359.



Truly colossal negative magnetoresistance in EuCd_2As_2 at low temperatures

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Weyl semimetals have attracted much attention due to their wide range of exotic properties predicted in theories. They represent an elegant example of the correspondence between condensed matter and high-energy physics because of its low-energy excitations. The Weyl fermions are massless particles (which obey the Weyl equation). Their energy bands show linear dispersion in the vicinity of nodes, termed the Dirac or Weyl points, as the three-dimensional analogue of graphene. The high mobility of charged Weyl fermions may find use in electronics and computing.

Layered antiferromagnet EuCd_2As_2 was predicted to be a Weyl semimetal. We shall present electrical transport and magnetic properties of a single crystal of EuCd_2As_2 with insulating behaviour. The samples exhibit VRH transport regime with colossal negative magnetoresistance of five orders of magnitude. Our findings cast a different light on previously reported interpretations of physics in EuCd_2As_2 .



Nb-Ni binary compounds in oxygen evolution reaction

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Hydrogen generation through electrochemical water splitting offers a sustainable and fossil-free solution for high quality hydrogen production. The oxygen evolution reaction (OER) is kinetically challenging due to complex processes with multielectron transfer comparing to hydrogen evolution reaction [1]. The feasibility of water electrolysis on large industrial scale is subject to develop highly efficient, stable, viable, and low-cost electrocatalysts for OER half-reaction. Recent studies have shown that transition metal catalysts (Ni, Co and Fe, etc.) as well as their compounds such as borides, carbides, nitrides and oxides, possess high OER activity and reasonable stability in alkaline environment aside from their relative low cost [2].

In our work, electrochemical behavior of Nb-Ni binary compounds in terms of their OER activity was investigated. Binary compounds NbNi₃ and Nb₇Ni₆ were synthesized via arc melting followed by homogenization annealing. The results of electrochemical studies in alkaline electrolyte, supported by extensive characterization of electrode material before and after electrochemical experiments, will be presented.

References:

- [1] N. T. Suen et al., Chem. Soc. Rev. **2017**, 46, 337.
- [2] L. Sun et al., Coord. Chem. Rev. **2021**, 444, 214049.



High-fluence ion irradiation for materials testing

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Energetic ion beams are commonly utilized to modify the properties and study accelerated radiation ageing of materials. In this contribution, we present our research on the application of high-energy ion irradiation as a surrogate for neutron radiation in nuclear reactors and experimental simulation of radiation conditions in Space. The ion beam laboratory of the Slovak University of Technology in Bratislava provides ion beams with energies up to 100 MeV. High fluence irradiations aim to investigate the effect of radiation environments on various materials from atomic-scale, particularly defect evolution, void and bubble formation followed by aggregation, transmutation – up to the macroscale, i.e. impact on engineering relevant properties. While the nanoscale defects are being probed by non-destructive analytical techniques such as positron annihilation spectroscopy, the macroscale properties by micro-mechanical testing techniques. The latest results on the effect of transmutation helium on the Eurofer97 steel and its Oxide Dispersion Strengthened variant are presented along with the capabilities of the laboratory.

Photoresponse behavior of Dye Sensitized Solar Cells

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The work reports about the behaviour of Dye Sensitized Solar cells. When exposed to 1.5 AM solar radiation generated by a solar simulator, the open circuit voltage (Voc) of the fabricated cells was measured as a function of time (for 30 days). The solar cell was fabricated using combination of three electrodes (one indium tin oxide (ITO) and two aluminium doped zinc oxide (AZO) under different conditions), two electrolytes (potassium iodide (KI) and lithium iodide (LiI)) and two dyes (Eosin Yellow and Ruthenium Red). A total of 12 solar cells were prepared using different combination of electrolyte, dye and electrodes. A variety of structural and elemental analyses were performed. XRD and Raman spectroscopy are used to characterize the deposited films and confirm the deposition of AZO films. The thickness and surface morphology of the films were measured using SEM. Elemental analysis was performed using EDX. Transparency of the film has been studied by US Vis spectrometry. Current-Voltage characteristic has also been studied with an aid of 4-point probe method. It was observed that AZO electrode with KI-EY and KI-Ru combination showed better results than the ITO electrode.

This work is in part supported by the scientific project „Intercalated transition metal dichalcogenides“ (HrZZ IP-2020-02-9666).

Characterization of Ga-Ni-Co-Cr-Fe-based multi-principal element alloys

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The effect of changes in gallium and nickel content on the microstructure and properties of $(\text{GaNi})_x\text{CoCrFe}$ ($x = 0.4, 0.7, 1.0, 1.3$ and 1.6) multi-principal element alloys was investigated. The $(\text{GaNi})_{0.4}\text{CoCrFe}$ alloy contains an FCC phase and when the ratio of gallium and nickel increases at the expense of the rest of the elements, a gradual change from FCC to BCC is observed. The hardness of alloys correlates with their phase composition. The density of the alloys gradually decreases as the ratio of gallium and nickel increases due to the low density of gallium. Some preliminary results of mechanical testing will also be presented.

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P-10

Phase transformation in decagonal Al-Cu-Rh quasicrystals induced by phasons

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We will present the results of the refinement of the decagonal Al-Cu-Rh quasicrystal structure model based on high-temperature data [1] using a new phason approach [2,3] and a generalized Penrose tiling (GPT) as a quasilattice [4]. A correlation between lattice parameters and the maximal residual electron density was observed, indicating a phase transformation at a temperature around 1083-1153 K. Phasonic disorder is modeled as a distribution of moments. Minima of values of moments are observed at 1083-1153 K, too, leading to the conclusion that the transition to a more stable phase is related to phason disorder.

The occurrence of the additional 5th atomic surface in GPT can be obtained by phasonic fluctuation of the ideal structure. In the refinement, we observed that the atomic distribution of the 5th atomic surface correlates with the stability of a structure at the temperature of approximately 1153 K, which could indicate the influence of the phason disorder on the stabilization of the structure [5].

References:

- [1] P. Kuczera, J. Wolny, W. Steurer, Acta Cryst. B 70 (2014) 306.
- [2] I. Buganski, R. Strzalka, J. Wolny, Acta Cryst. A 75 (2019) 352.
- [3] I. Buganski, R. Strzalka, J. Wolny, J. App. Cryst. 53 (2020) 904.
- [4] M. Chodyn, P. Kuczera, J. Wolny, Acta Cryst. A 71 (2015) 161.
- [5] I. Bugański, R. Strzalka, J. Wolny, Acta Cryst. A 78 (2022) 402.

Emergence of intercalated transition metal derived bands near the Fermi level of (Co, Ni)_{1/3}NbS₂

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Transition metal intercalated NbS₂ have been studied for decades, yet their complexities remain to be solved. The host 2H-NbS₂ is a superconductor below 6 K. Intercalation of transition metal atoms suppresses the superconductivity and introduces magnetic ordering. A series of 3d transition metal intercalated NbS₂ forms in a certain concentration M_{1/3}NbS₂ (M: 3d transition metal), and their magnetic structure depends on a selection of transition metals. Both Co_{1/3}NbS₂ and Ni_{1/3}NbS₂ exhibit antiferromagnetic ordering in ab-planes at T_N~26 and 90 K, respectively. We performed angle-resolved photoelectron spectroscopy on Co_{1/3}NbS₂ and Ni_{1/3}NbS₂ to study their electronic structure. The observed band dispersion of both compounds showed the similar features as 2H-NbS₂ bands. However, a clear distinction from 2H-NbS₂ bands was observed in the vicinity of the Fermi level as a shallow electron pocket originating from the intercalated atoms.

This work is in part supported by the scientific project "Pressure- and Temperature-driven Phase transitions in Strongly Correlated Electron Systems (PaT PiSCES)"HrZZ UIP-2019-04-2154

P-12

Synthesis and characterization of magnetic transition metal chalcogenides

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Two dimensional magnetic materials have been gaining attention as potential candidates for spintronic devices. Among them, transition metal dichalcogenides intercalated by magnetic atoms have been intensively studied due to their structural diversity, and rich electrical and magnetic behaviors. One of the most interesting series of materials is $M_x\text{NbS}_2$ (M: 3d transition metal). Intercalated ions occupy octahedral vacancy sites in the van der Waals gaps and form super-lattice structures. We have grown $\text{Co}_{1/3}\text{NbS}_2$ and $\text{Ni}_{1/3}\text{NbS}_2$ single crystals by chemical vapor transport method using iodine as a transport agent. The grown crystals have been characterized by powder x-ray diffraction, magnetic and electrical transport measurements. Both crystals formed into a hexagonal structure (space group: $P6_322$). $\text{Co}_{1/3}\text{NbS}_2$ and $\text{Ni}_{1/3}\text{NbS}_2$ showed antiferromagnetic ordering at $T_N \sim 25$ and 91 K, respectively, that were in good agreement with previous studies [1, 2]. Details of the synthesis and analysis will be discussed in the poster presentation together with our latest progress in the growth of transition metal phosphides samples (Mn_2P , MnP and Fe_2P).

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References:

- [1] P. Popčević et al., Physical Review B **105**, 155114 (2022).
- [2] R. H. Friend et al., Philos. Mag. 35, 1269 (1977).

Contributions to the understanding of thermal and electronic transport in complex metallic compounds: from periodic to quasi-periodic crystals

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Building on the expertise of the investigation (measuring, analyzing and interpreting) of thermal and electrical transport in the field of strongly anisotropic inorganic quasi-one-dimensional periodic systems [1-3], with our collaborators at CRTB in Grenoble we expanded our interest to investigation of the transport and magnetic properties of quasiperiodic systems [4, 5]. In cooperation with the NMR group of professor J. Dolinšek (IJS, Ljubljana, SLO) we have intensified, the initiated research of quasiperiodic systems, within the framework of bilateral CRO-SLO cooperation. The collaboration was very motivating and fruitful, both educationally and scientifically. It resulted with successful completion of several doctoral theses on both sides. The results of this collaborative complementary research have been presented at numerous conferences, workshops and schools organized within as well as wider than the framework of EU cooperation: first the EU project Complex metallic alloys (CMA) and then within the EU network C-MAC (today ECMetAC). On the occasion of Prof. J. Dolinšek 65 birthday, we will present some highlights of our contributions to the understanding of quasi-periodic systems, presented in refs. [6-12].

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References:

- [1] A. Smontara, et.al, J. of Phys.: Cond. Matter 4 (1992), 3273;
- [2] A. Smontara, et. al., Phys. Rev. B 48 (1993), 4329
- [3] A. Smontara, et. al., Phys. Rev. Lett. 77 (1996), 5397
- [4] A. Bilušić, et.al., Mat. Sci. Eng. A, 294(2000), 711
- [5] A. Bilušić, et.al, Vacuum 61 (2001), 345
- [6] A. Bilušić, et.al., J. Alloys and Comp 342 (2002), 413
- [7] J. Dolinšek, et al., Phys. Rev. B 72 (2005), 064208
- [8] Ž. Bihar, et.al., J. Alloys and Compds 407 (2006), 65
- [9] A. Smontara, et.al, Phys. Rev. B 78 (2008), 104204
- [10] P. Popčević, et al., Phys. Rev. B 81 (2010), 184203
- [11] M. Bobnar, et.al. Phys. Rev. B 85 (2012), 024205
- [12] P. Popčević, et. al., in preparation

Tuning thermal conductivity of hydrogen fuel cell catalyst films

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Catalyst films (polymer electrolyte membranes) are prepared at Faculty of Science, University of Split and successfully implemented into hydrogen micro fuel cells with promising performance. Catalyst films are to be modified by addition of noble metal-based multimetallic nanoparticles with the aim of increasing dry film electron conductivity, proton and lateral heat conductivity thus improving fuel cell efficiency and longevity.

We present the experimental setup for automating high temperature electrical and thermal measurement in arbitrary atmosphere (Argon, vacuum). 3ω measurement technique is chosen for thermal measurements and can be applied to bulk amorphous solids, crystals and amorphous films tens of microns thick [1]. Micro heaters are fabricated by photolithography onto a measured material. AC current is passed through the micro heater with frequency ω , which induces local heating of the material as a function of 2ω . Resistance depends linearly on the temperature change. Voltage differential across the metallic heater is measured. The third harmonic of the voltage differential contains information on the thermal properties of the material. Electrical and thermal measurements are automated through software (LabVIEW).

Reference:

- [1] David G. Cahill, Review of Scientific Instruments 61, 802 (1990)

Influence of surface oxidation on the OER activity and stability of ZrNi and ZrCo

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Hydrogen production by mean of water electrolysis is a promising strategy to efficiently store energy from intermittent renewable power sources. The oxygen evolution reaction (OER) occurring at the anode is kinetically slow and reduce the overall efficiency of current electrolyzers. The discovery of new anode material possessing enhanced OER activity is therefore of tremendous importance nowadays. In addition, the electrode material must also show high operating stability to withstand the harsh industrial conditions which involve high current densities, highly concentrated alkaline electrolyte and elevated temperatures [1].

In our approach a controlled oxidation of bulk intermetallics material to form a thin oxide layer at the surface was carried out. In this way, the formation of a catalytically active oxide layer, that will at the same time protect the conductive intermetallic underneath and preserve sufficient electrical conductivity of the electrode was attempted. The present contribution will focus on the results obtained by applying this approach to the rare-metal free ZrNi and ZrCo compounds. The OER activity and the stability over time of electrodes which have been treated under different oxidation conditions will be compared and discussed.

Reference:

[1] M. Chatenet et al., Chem. Soc. Rev. (2022) 51, 4583.