European C-MetAC

European Integrated Centre for the Development of New Metallic Alloys & Compounds

Book of Abstracts

of the

European C-MetAC Days 2024

15th annual meeting

November 25 – 28, 2024
Zagreb CROATIA

ECMetAC Days 2024

BOOK OF ABSTRACTS

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ECMetAC Days 2024, Zagreb, Croatia, November 25 – 28, 2024

15th annual meeting of the European Integrated Centre for the Development of New Metallic Alloys & Compounds

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Dear participants

of ECMetAC Days 2024, we warmly welcome you to Zagreb, the capital of Croatia. This year marks the 15th edition of the ECMetAC Days conference series, organized annually by the European Integrated Center for the Development of Metallic Alloys & Compounds (ECMetAC, https://www.ecmetac.eu/). While this is the second time the conference is being hosted at the Institute of Physics in Zagreb (the first was in 2014, under the name C-MAC Days before the rebranding to ECMetAC), it is now co-organized by the Department of Physics, Faculty of Science, University of Zagreb, and the Institute of Physics.

The topics covered in the conference series include the formation, stability, synthesis, and structural and chemical characterization of metallic materials, as well as their physical, chemical, and mechanical properties. Additional focus areas include surfaces and thin films, catalysis, theoretical developments, applications, and emerging frontiers in the field.

The conference program offers an excellent opportunity to gain insights into the latest results and cutting-edge advancements in the fields of 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.

As mentioned earlier, this year marks the 15th anniversary of the ECMetAC and the 20th anniversary of the CMA NoE project, which led to the founding of the ECMetAC. To commemorate this milestone, a special session dedicated to the ECMetAC 's development will be held to honor its legacy.

We wish you a pleasant stay in Zagreb, and fruitful ECMetAC Days 2024.

On behalf of the organizing committee
Petar Popčević & Mario Novak

Organizers:
Mario Novak & Petar Popčević

Local organizing committee:
Ana Smontara
Neven Barišić
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Organizing Institutions:
Institute of Physics and University of Zagreb Faculty of Science

Zagreb, Croatia, 2024

Conference program

ECMetAC Days 2024 program

Monday, November 25

Venue: Hotel Dubrovnik,
Conference room:
BAN FRANKOPAN

***ED&I Workshop* (Magdalena Wencka)** - Innovative researcher: how to make an impression when presenting data.	
15:00 – 16:00	Zoom with **Joanna Janowicz** (speech and Q&A)
16:00 – 16:15	Coffee break
16:15 – 17:00	Interviews with ECMetAC scientists of different generations
17:00 – 17:30	Training

Venue: Hotel Central

16:00 – 20:00	Registration
18:00 – 20:00	Welcome reception

Tuesday, November 26

Venue: Institute of Physics

8:45 Opening
Welcome address by director of Institute of Physics ***Osor S. Barišić****, head of the Physics department of the Faculty of Science* ***Ivan Kupčić*** *and CEO of the ECMetAC* ***Julian Ledieu***

Session 1	Chair: **Ana Smontara**
9:00	**Jean-Marie Dubois** (Ljubljana & Nancy) *A quick look backwards to the origin of the ECMetAC network*
9:30	**Yuri Grin** (Dresden) *Structural complexity and transverse Seebeck effect*
10:05	**Julian Ledieu** (Nancy) *The ECMetAC current status and opportunities*

10:20 Coffee break

Session 2	Chair: **Iryna Antonyshyn**
10:50	**Eteri Svanidze** (Dresden) *Chemical facets of superconductivity in UTe_2*
11:20	**Ana Akrap** (Zagreb) *Magnetism and band structure of $EuCd_2As_2$*
11:40	**Rachel Nixon** (Dresden) *Superconductivity of transition metal mercurides*
12:00	**Nives Štrkalj** (Zagreb) *Exploring (multi)ferroic order at interfaces of oxide heterostructures*
12:20	**Mirta Herak** (Zagreb) *Magnetoelectric effect and symmetry in topological antiferromagnet Cu_3TeO_6*

12:40 Lunch

Session 3	Chair: **Petar Popčević**
14:10	**Neven Barišić** (Zagreb & Vienna) *High-Tc Cuprates: From Synthesis to Phenomenology*
14:30	**Janez Dolinšek** (Ljubljana) *Physical properties of intermetallic phases: The Ljubljana–Zagreb cooperation*
14:50	**Peter Gille** (München) *Czochralski single crystal growth of intermetallics for studies of electronic and magnetic properties*
15:10	**Ante Bilušić** (Split) *Electric properties of WN_x in magnetic field*

15:30 Coffee break

Session 4	Chair: **Marc Armbrüster**
16:00	**Marc Heggen** (Jülich) *In-situ transmission electron microscopy study of nanoparticle alloy catalysts*
16:30	**Iryna Antonyshyn** (Berlin) *Interplay between experiment and theory: Al-Pt compounds*
16:50	**Jacob Wright** (Dübendorf) *Asymmetric Heterogeneous Catalysis of Chiral Molecules on PdGa{111}*
17:10	**Florian Brix** (Nancy) *Structure of an Ultrathin Oxide on InPd(100) and machine-learning assisted catalysis study*
17:30	**Anton Kabaši** (Split) *Thermal transport measurement in Nafion thin films: the 3-omega method*

18:00 ***Poster session***

19:00 EB meeting

Wednesday, November 27

Venue: Institute of Physics

Session 5	Chair: **Magdalena Wencka**
9:00	**Andreja Jelen** (Ljubljana) *Correlating multiscale structural properties to magnetic characteristics of HEAs*
9:30	**Julia Petrović** (Ljubljana) *Physical properties of $Ce_xNdPrSm$ (x = 0.01-1.5) medium-entropy alloys*
9:50	**Primož Koželj** (Ljubljana) *$CeFe_9Si_4$: Magnetism in an intermetallic compound with transition metal and rare earth atoms*
10:10	**Priyanka Reddy** (Vienna) *High-entropy magnetism of murunskite*

10:30 Coffee break

Session 6	Chair: **Roland Widmer**
11:00	**Yannick Champion** (Grenoble) *Entropy and Structure of high entropy metallic alloys*
11:20	**Laetitia Laversenne** (Grenoble) *High entropy alloys for solid state storage of hydrogen*
11:40	**Janusz Tobola** (Krakow) *Interplay of chemical disorder and local structural dislocations in superconducting high-entropy alloys*
12:00	**Vincent Fournée** (Nancy) *Structural and magnetocaloric properties in rare-earth free high-entropy alloys*
12:20	**Emil Babić** (Zagreb) *Electronic structure of compositionally complex alloys: challenges and prospects*

12:40 Lunch

Session 7	Chair: **Hem Raj Sharma**
14:10	**Gabriel Kuderowicz** (Krakow) *Study of lattice dynamics and electron-phonon interaction in SnTe:In and PbTe:Tl*
14:40	**Émilie Gaudry** (Nancy) *Hydrogen, oxygen, and lead adsorbates on $Al_{13}Co_4$(100): accurate potential energy surfaces at low computational cost by machine learning and DFT-based data*
15:00	**Marek Mihalkovič** (Bratislava) *Spontaneous metal-semiconductor phase transition in atomistic simulations of liquid and amorphous Germanium*
15:20	**Kacper Pryga** (Krakow) *Electronic structure and transport properties of Fe doped γ CuI – complex interplay of Fe impurities*
15:40	**Joanna Marciniak** (Poznan) *Giant magnetocrystalline anisotropy energy in Fe–Co alloy under uniaxial compression: first-principles prediction*

16:00 Coffee break

Session 8	Chair: **Thomas Seyller**
16:30	**Johannes Roth** (Stuttgart) Impact of hyperthermal oxygen on alumina surfaces investigated by molecular dynamics simulations
16:50	**Oksana Karychort** (Dresden) New samarium and ytterbium iron arsenides: crystal structure and physical properties
17:10	**Sylwia Nowak** (Krakow) Determination of the second order plastic incompatibility stresses in deformed hexagonal materials

17:30	**Radovan Bujdák** (Trnava) Novel oxo-peroxide and oxo-superoxide phases in Ni-O binary system
17:50	Closing remarks (**Ronan McGrath, Mario Novak**)

19:30 gala dinner *Venue: Hotel Central*

Thursday, November 28

Venue; Institute of Physics

8:00	Science Board Meeting
9:45	Coffee break
10:15	Governing Board Meeting and General Assembly

12:00 Lunch

List of posters

Poster session	Tuesday, November 26, 18:00 - 20:00 *Venue: Institute of Physics*
P1	**Luka Akšamović** (Vienna) *High Tc cuprates: fabrication of 2D devicess*
P2	**Ahowd Alfahad** (Liverpool) *Surface Atomic and Structure of In_3Ni_2 Intermetallic*
P3	**Mario Basletić** (Zagreb) *Magnetotransport properties of selected high entropy alloys*
P4	**Ireneusz Buganski** (Krakow) *Synthesis and structural analysis of ZnMgEr P-type quasicrystals*
P5	**Diana Fabušová** (Trnava) *Theoretical investigation of novel palladium suboxide Pd2O*
P6	**Vincent Fournée** (Nancy) *Single crystals of Nd-Fe-B permanent magnets and UHV surface investigation of their surface structure.*
P7	**Simon Kümmel** (Stuttgart) *Investigation of excitation-induced non-thermal effects in semiconductors, metals and alloys*
P8	**Go-Woon Lee** (Daejeon) *XRD/FIB/SEM characterization of the $Ce_xPrNdSm$ high-entropy alloys*
P9	**Jože Luzar** (Ljubljana) *Physical properties of supersilent $(GaNi)_xCoCrFe$ high-entropy alloys*
P10	**Wilfred Bajoun Mbajoun** (Nancy) *Single-grain re-engineered Nd-Fe-B permanent magnets.*
P11	**Peter Mihor** (Ljubljana) *Magnetic softness and vanishing magnetostriction in high-entropy alloys $(GaNi)_xCoCrFe$ ($x = 0.4–1.6$)*
P12	**Seyed Ashkan Moghadam Ziabari** (Zagreb) *Temperature dependent electrical resistivity measurement of Mn_2P under high pressure*

P13	**Jana Mužević** (Zagreb) *Single crystal synthesis of doped murunskite*
P14	**Juraj Nálepka** (Trnava) *Characterization of lightweight TiAlSc multi-principal element alloy*
P15	**Nikolina Penić** (Zagreb) *Role of the functional group effect in tailoring rare supramolecular copper(II) magnetic architectures*
P16	**Gaurav Pransu** (Zagreb) Synthesis and Characterization of Magnetic and Transport Properties in Intercalated TMDs
P17	**Pavol Priputen** (Trnava) *Thermal expansion of CoFeNiCu-based multi-principal element alloys*
P18	**Peter Richter** (Chemnitz) *Growth and characterization of CoCrFeNi on $LaAlO_3$ substrates*
P19	**Petar Sačer** (Zagreb) *Quantum oscillations in Sn-doped BST2S topological insulator*
P20	**Wojciech Sas** (Zagreb) *The study of electronic transport properties of transition metal dichalcogenides under uniaxial pressure using a piezo-driven stress cell*
P21	**Ana Smontara** (Zagreb) *Institute of Physics – From participation in the European Network of Excellence, NoE CMA to the partner institution of the European Integrated entre (EC-MetAC)*
P22	**Josipa Šćurla** (Split) *Magnetotransport in crystal rutile and anatase*
P23	**Stanislav Vrtnik** (Ljubljana) *Spin-glass phase in Zn-Mg-RE (RE = Er, Tm) quasicrystals*

Monday,

November 25, 2024

Innovative researcher: how to make an impression when presenting research data

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„Innovative researcher: ...“ – a series of workshops allows researchers from our Network to enrich their experience in new perspective belonging to experts from outside the field of science as well as scientists. This time we will focus on public speaking and skills of presenting scientific data. In the first part of our meeting, we will meet with Joanna Janowicz who is an expert on public speaking in business. She is a creator and organizer of her own unique cycle of meetings dedicated to speeches and effective communication with an audience that are held on a roof of the ENEA football stadium in Poznań in Poland and are entitled „Extreme Public Speaking“. Joanna will teach us how to eliminate harmful stress and fear that appear standing in front of the audience and how to communicate with our recipients. We will also have an opportunity to get hints from scientists of different generations, who sharing their secrets, help us to make an impression when presenting research data. At the end, a practical part will finalize our workshop.

Tuesday,

November 26, 2024

A quick look backwards to the origin of the ECMetAC network

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At the beginning of the 21st century, around 2002, quite a few of us had been working on quasicrystals for more than a decade. This discovery by Dan Shechtman and few others had been deeply influencing our researcher's life and we were all greedy to establish the growing field of quasiperiodic crystals as firmly as possible. Many were prone to work on the crystallography of these new materials and its exotic higher dimensional spaces. Few were more attracted by their properties and potential applications. Based on rather scarce explorations of the phase diagrams, it was obvious that in a given system, when it existed, the quasicrystal was only the tip of a deeply underlying iceberg, yet invisible and unknown, of many crystals – approximants and resembling crystals – that although periodic were of great fundamental, if not practical, importance.

At that time, I was often interacting with my great colleague, Prof. Dr Knut Urban, one of the most famous electron microscopists worldwide. He was leading the group of German scientists who worked on quasicrystals, and was the first to embrace the importance of the hidden iceberg.1 In parallel, I was in charge of a European project focusing at potential applications of quasicrystals. Another great scientist from Switzerland, Prof. Dr Louis Schlapbach, well known for his pioneering contributions to hydrides and hydrogen in metals, was also involved in this EC project. We decided to join our efforts to apply to a so-called European Network of Excellence (NoE). The concept of NoEs had been conceived by the former French prime minister, Mrs Edith Cresson, when she was in charge of science in Brussels. After a short period of embarassment, we decided to coin the CMA acronym

for Complex Metallic Alloys NoE. CMA is still used in literature to address the broad range of complex intermetallics.

Our application file was good: the project was selected and a budget of 7,200,000 euros allocated. The NoE coordinated the efforts of about 400 scientists located in 12 Euroepan countries. It had strong links with few labs in the USA, Japan, China, and Brazil. It took 2 years to negotiate the details of the contract with the EC, but the kick-off could take place in Luxembourg in 2005. The project lasted for 5 years until 2010. One of its mandatory outcomes was the creation of a permanent research body, and this is why and how the ECmetAC network was born. I will try to analyse few other products of the CMA NoE, namely the Euroschool, which is also still active, the gender mainstreaming, and the way the network was actuated. Developments beyond the shutdown of the CMA NoE will be addressed by the colleagues in charge.

[1] K. Urban, M. Feuerbacher, Structurally Complex Alloy Phases, Journal of Non-Crystalline Solids, **334&335**, 143 (2004).

Structural complexity and transverse Seebeck effect

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Transverse Seebeck effect appears perpendicular to the heat direction in a system with anisotropic Seebeck effect. This possibility was pointed out already by W. Thomson [1]. The condition of appearence of anisotropic Seebeck effect is anisotropy of the materials. There are not very much examples of such behaviour. Beside known cases of thin films of Bi [2], binary CdSb [3], in the last decades anisotropy of Seeback effect was reported, e.g., for Re_4Si_7 [4], $CsBi_4Te_6$ [5], several two-phase materials, a.o. Co_2MnGa/Si [6], $Bi_2Sr_2CaCu_2O_8$ [7] and also for the CMA *o*-$Al_{13}Co_4$ [8].

The anisotropy of the multi-phase materials originates from the unitary axis construction. For the single phase materials, the anisotropy may base on structure modulations, or on the partial violation of the translational symmetry in a plane. The transverse Seebeck effect in *o*-$Al_{13}Co_4$ i.e. single-phase materials containing two metals, was demonstrated recently by a cooperative research within ECMAC and Institute of Thermoelelctricity NAN Ukraine [9].

[1] W. Thomson. in: Mathematical and physical papers, Univ. Press Cambridge, 1882, p. 266.
[2] S. Cho *et al.*, J. Appl. Phys. **88**, 808 (2000).
[3] S.L. Korolyuk *et al.*, Sov. Phys. Semicond. **7**, 502 (1973).
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[5] D.-Y. Chung *et al.*, JACS **126**, 6414 (2004).
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[7] W.M. Huber *et al.*, Appl. Phys. A **64**, 487 (1997).
[8] J. Dolinšek *et al.*, Phys. Rev. B **79**, 184291 (2009).
[9] Yu. Grin, L. I. Anatychuk, P. Gille, M. Havrylyuk, M. Krnel. ICT 2023, Krakow, Book of Abstracts (2024).

The ECMetAC current status and opportunities

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This year marks the 15th anniversary of the foundation of ECMetAC, a long-lasting entity of the Network of Excellence on Complex Metallic Alloy started in 2005. With more than twenty Institutes or laboratories involved, this European Integrated Center provides world leading cutting edge knowledge in material science and material science simulation of complex systems. The main objectives of the consortium are to promote collaborative research, combining both experimental and theoretical approaches, in the field of metallic alloys and compounds at a European level to reach excellence. This ECMetAC Days organized this year in Zagreb would be a great opportunity to introduce the current status of ECMetAC, the different research and activity domains, the dedicated Euroschool organized annually along with the present and future opportunities associated with such European Integrated Center.

Chemical facets of superconductivity in UTe_2

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Unconventional superconductor UTe_2 has attracted much attention since its discovery in 2019. [1,2] Still, many questions remain regarding the intrinsic crystal structure and its affect on the physical properties. In particular, it has been shown that the crystals of UTe_2 can be grown in several different ways – Te-flux, [1] chemical vapor transport, [3,4] and salt flux. [5] While previous reports [3,6–8] have related the differences between T_c, residual resistivity ratio, shape and height of the specific heat anomaly to the particular features of the synthesis route, the complete understanding of underlaying chemical features that cause these differences remains unknown. I will discuss a comprehensive review on the sample-dependence of UTe_2 and provide microscopic insight into the origin of differences, reported so far for this peculiar system.

[1] S. Ran *et al.*, Science **365**, 684 (2019).
[2] D. Aoki *et al.*, J. Phys. Condens. Matter **34**, 243002 (2022).
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[5] H. Sakai *et al.*, Phys. Rev. Mater. **6**, 073401 (2022).
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[8] Y. Haga, *et al.*, J. Phys. Condens. Matter **34**, 1 (2022).

Magnetism and band structure of $EuCd_2As_2$

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$EuCd_2As_2$ has emerged as a topological material where magnetism may produce strong effects. This compound has been understood as a candidate Weyl semimetal, based mostly on *ab initio* calculations, transport and photoemission measurements. I will present our recent results on samples in which we control the carrier concentration through chemical synthesis. We find magneto-optical evidence of a sizeable band gap, remarkably sensitive to the local Eu magnetism. Our results contradict the current consensus on the ground state of this compound, bringing into question its topological nature.

Superconductivity of transition metal mercurides

[1,*]R. Nixon, [1]Y. Prots, [1]M. Krnel, [1]N. Zaremba, [1]M. Schmidt, [1,2]L. Akselrud, [1]M. König, [1]Y. Grin and [1]E. Svanidze

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Mercury-based materials have been of interest for decades [1-3]. Our current work is inspired by an unconventional superconductor BeAu , with its noncentrosymmetric crystal structure giving rise to its peculiar properties [4-6]. In our search of isostructural mercury-based materials, we turn to PdHg, which shares the same space group of B20-type structure [7]. We further investigate other Pd- and Pt-mercurides, motivated by their complex binary phase diagrams [8-9]. As is the case for many other mercury-based systems, we rely on specialised laboratory conditions for the synthesis and characterisation of our materials [10-12]. Our work aims to reveal the properties of known phases, discover new phases, and map out the phase diagrams of these challenging materials.

[1] J. Sappl, *et al.*, Crystals **7**, 352 (2017).
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[10] Y. Prots, *et al.*, Inorg. Chem. **61**, 15444 (2022).
[11] K. Witthaut, *et al.*, ACS Org. Inorg. **3**, 143 (2023).
[12] Y. Prots, *et al.*, Phys. Rev. B **106**, L060412 (2022).

Exploring (multi)ferroic order at interfaces of oxide heterostructures

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Oxide heterostructures with ferroic materials present a promising platform for emergent interfacial phenomena. We investigate conventional exchange bias (EB) in ultra-thin ferroelectric (FE) $BaTiO_3$ (BTO) and ferromagnetic (FM) $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) bi-layers, without the presence of an antiferromagnetic (AFM) material. The EB arises from electronic orbital reconstruction at the FE-FM interface due to ferroelectric polarization, achieving a maximum of ~42 Oe for 9 unit cells of BTO. This thickness balances the critical threshold for ferroelectricity and strain relaxation. Furthermore, the LSMO layer needs to be thick enough to sustain both FM layer and polarization-induced AFM spin configuration at the LSMO-BTO interface, yet as thin as possible to enable the EB loop shift. Our results, supported by X-ray magnetic circular dichroism, scanning transmission electron microscopy, and density functional theory calculations, reveal that the EB effect originates from interfacial AFM spin configuration in LSMO, driven by FE-induced d-orbital modifications in interfacial Mn ions. This work demonstrates effective engineering of interfacial EB coupling in artificial multiferroics through controlled FE polarization. Even further, it invites investigation into complex polar and magnetic textures in (multi)ferroic oxide heterostructures.

Magnetoelectric effect and symmetry in topological antiferromagnet Cu_3TeO_6

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Antiferromagnets (AFMs) are important candidate materials for future spintronic devices. Zero net magnetization and terahertz dynamics could lead to an increase in information processing and storage by several orders of magnitude. Unprecedented energy efficiency could be achieved in magnetoelectric AFMs where magnetic states are controlled by voltage, or by exploiting magnons to carry spin instead of electric currents. The propagation of topologically protected magnons is found to be robust against perturbations. Cu_3TeO_6 is a topological AFM material with unique vortex sharing hexagon magnetic lattice. Recently, we reported a linear magnetoelectric effect in the AFM state of Cu_3TeO_6 through static polarization measurements [1]. We show that an applied magnetic field induces spin reorientation and quantitatively determine the accompanying change in magnetic symmetry, which is relevant for the magnetoelectric and topological properties of this material. Our findings establish Cu_3TeO_6 as a promising material for studying the interplay of several key spintronic-related phenomena.

[1] V. Kisiček *et al.*, Phys. Rev. Lett. **132**, 096701 (2024).

High-Tc Cuprates: From Synthesis to Phenomenology

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Superconductivity is a property exhibited by certain materials, enabling the flow of electricity without dissipation. Understanding this phenomenon wherever it occurs is not only crucial conceptually but also holds immense technological potential. Therefore, it is not surprising that high-Tc cuprates are among the most intensively studied correlated materials. Nonetheless, fundamental questions about their main phases and regimes, as well as the transitions between them, remain unanswered. This is mainly due to the complexity of these materials that renders the extraction of intrinsic properties difficult.

We addressed this challenge by identifying $HgBa_2CuO_{4+\delta}$ as a model cuprate compound, which motivated an extensive effort in the synthesis high quality crystals [1]. Comprehensive experimental studies, conducted on meticulously characterized materials, and through a comparison with data obtained for other cuprates revealed a set of remarkably simple universalities. The most important of them are that the effective mass and scattering rate of itinerant charges remain essentially unchanged across the phase diagram [2,3,4]. This has led to a straightforward determination of carrier density, revealing a second localized electronic subsystem [4,5,6]. The delicate balance between these subsystems is attributed to a change in the nature of the planar CuO 3d-2p bond from ionic to covalent [6].

Finally, we established that the itinerant Fermi-liquid charges become superconducting, while the localized charge provides the superconducting "glue" [4,5,6]. With this, we have greatly demystified the physics of these fascinating compounds.

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Physical properties of intermetallic phases: The Ljubljana–Zagreb cooperation

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Since the beginning of the 21st century, the research of intermetallic phases has moved from simple metallic alloys and compounds based on one principal element to multi-component intermetallic phases with many principal elements. Such phases include quasicrystals, complex intermetallic phases with giant unit cells, metallic glasses and high-entropy alloys. These phases sometimes show combinations of physical-mechanical properties that are absent in conventional alloys that are based on a single majority element. Such "smart" combinations are a combination of an electrical conductor with a thermal insulator, a combination of strength and ductility and a combination of magnetic softness and vanishing magnetostriction in ferromagnetic alloys. The materials from the above classes were investigated jointly by the group from Jožef Stefan Institute, Ljubljana, Slovenia and the group of dr. Ana Smontara from the Institute of Physics, Zagreb Croatia. This research has resulted in 47 joint publications in the period 2000 – 2014, and the results will be reviewed in the talk

Czochralski single crystal growth of intermetallics for studies of electronic and magnetic properties

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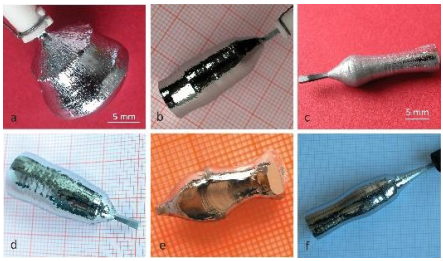
Czochralski's famous method of single crystal pulling from a melt has been used for a variety of intermetallic systems under conditions of high-temperature solution growth. Successful growth could be achieved from Al-rich, Ga-rich and In-rich solutions and will be discussed in the talk with special emphasis on the question what is common and what is different with respect to the growth process.



Examples of Czochralski-grown intermetallic single crystals: (a) $FeGa_{3-x}Ge_x$, (b) Ga_3Ni_2, (c) $Al_{13}Co_4$, (d) PdGa, (e) $Al_{13}(Fe,Cr)_4$, and (f) a decagonal $Al_{72}Co_9Ni_{19}$ quasicrystal.

Growth of decagonal Al-Co-Ni and Al-Co-Cu as well as periodic crystals of $Al_{13}Co_4$, $Al_{13}Fe_4$, $Al_{13}(Fe,Cr)_4$, $Al_{13}(Fe,Ni)_4$, Ga_3Ni_2, PdGa, Pd_3Ga_7, $PdGa_2$, InPd, and Pd_3In_7 will be compared. These intermetallic phases very much vary in the the number of atoms in their unit cells. What has been found in all these experiments is the need of a fully metal-sealed vacuum system for the growth chamber and extremely low pulling rates when compared to usual Czochralski crystal growth procedures. Sample preparation for studies of electronic transport and magnetic properties is shortly presented as well.

Electric properties of WN_x in magnetic field

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Due to their mechanical and electrical properties, transition metal nitrides have potential for the development of new cutting tools and electrode materials. We will present the electrical resistance of tungsten nitride WN_x at low temperatures in magnetic fields, where x is the ratio of nitride to metal. It shows a semiconductor-like behaviour where the resistivity increases from 300 K to 2 K by almost five orders of magnitude. The electrical conductivity at low temperatures is proportional to $T^{-2/5}$, indicating the presence of a Coulomb gap at the Fermi level [1]. The magnetoresistance at 2 K is positive and reaches 20% at a magnetic field of 10 T. When heated, it changes sign and becomes lower, e.g. -5 % at 50 K.

[1] M. M. Fogler, S. Teber, and B. I. Shklovskii, Phys. Rev. B **69**, 035413 (2004).

In-situ transmission electron microscopy study of nanoparticle alloy catalysts

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Nanoparticle alloys are highly important materials in various applications, such as catalysis. Here we present an overview of recent microstructural studies at the Ernst Ruska-Centre on the formation, structural evolution, and degradation behavior of nanoparticle alloys using in-situ electron microscopy. For example, octahedral shaped Pt-Ni-based alloy nanoparticles have become highly attractive fuel-cell catalysts due to their extraordinary high activity for the oxygen-reduction-reaction. Furthermore, intermetallic PdZn nanoparticles are highly selective catalysts in Methanol steam reforming. In both cases, a deep understanding on their atomic-scale structure, structural evolution during the synthsis process, and degradation behavior is essential for the rational design of advanced nanoparticle catalysts with high activity, selectivity, and long-term stability.

Interplay between experiment and theory: Al-Pt compounds

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Modification of electronic structure of Pt via formation of Al-Pt compounds was the main idea to enhance it's activity towards oxygen evolution reaction (OER) with simultaneous preservation of Pt stability features upon oxidative reaction conditions.

Study on Al-Pt compounds as OER electrocatalysts clearly reveals: (i) the instability and noticeable leaching of Al in case of Al_4Pt and $Al_{21}Pt_8$; (ii) enhanced (compared to elemental Pt) OER activity of Al_2Pt and Al_3Pt_2 compounds with obvious activation after electrochemical pre-treatments, (iii) OER activity of Al_3Pt and Al_3Pt_5 comparable with elemental Pt [1]. Upon OER, Al-Pt compounds do not maintain their structural and electronic properties on the surface and near-surface region due to the Al leaching and surface rearrangement. Tracking such changes during the reaction using different spectroscopy techniques requires the use of reference values, which are scarce or non-consistent in the literature. Therefore, systematic HAXPES study on Al-Pt compounds was carried out and delivered thought-provoking results, requiring support of extensive computational analysis on these compounds [2]. Clear correlation between experimentally obtained Pt 4*f* core level shifts and calculated negative charges of Pt as well as occupancy of Pt 5*d* orbitals was drawn in this study.

[1] A.M. Barrios Jiménez, *et al*., Dalton Trans. **52**, 1433 (2023).
[2] I. Antonyshyn, *et al*., Phys. Chem. Chem. Phys. **25**, 31137 (2023).

Asymmetric Heterogeneous Catalysis of Chiral Molecules on PdGa{111}

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Chirality is an essential ingredient in the function of our biological world. Nearly 50% of new agrochemical products since 2007 contain at least one chirality center in the molecule. We further find that chirality is essential to many of the physiological processes in our bodies, such as smell and drug adsorption, as the proteins in our bodies are chiral. There is a clear and growing demand for the efficient production of enantiopure chemicals that can be aided by better understanding the atomistic-scale physics involved in their creation. PdGa, an intermetallic compound of space group No. 198, couples an intrinsic chirality with stability and metallicity – ideal properties for catalyzing on-surface asymmetric reactions. It is therefore an excellent candidate to study the role of chirality transfer, along with ensemble and ligand effects, in promoting enantioselectivity. For this task, we investigate the adsorption and reactions of phenanthrene-based molecules on atomically well-defined PdGa{111} surfaces under ultra-high vacuum (UHV) with scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM).

Structure of an Ultrathin Oxide on InPd(100) and machine-learning assisted catalysis study

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In this work, we investigate the surface structure and catalytic properties of an ultrathin oxide film on InPd(100), with a focus on its application in CO_2 hydrogenation to methanol. A 1 × 7 surface has been identified via Low-Energy Electron Diffraction (LEED) and studied with theoretical modeling using a genetic algorithm (USPEX) [1,2]. We identify a stable oxygen-induced surface reconstruction at low oxygen coverage.

This reconstruction shows a 1 × 7 periodicity with varying oxidation states of In^{2+}, In^{3+}, and In^{4+}. These oxidation states provide a wider surface's ability to adsorb molecules, as confirmed by machine learning-assisted adsorption energy calculations. A model of machine learning graph-neural network has been trained on previous calculated surfaces reconstructions and adsorption configurations and used to compute reaction barrier energies [3].

Our findings suggest that this reconstructed surface presents unique catalytic properties, which differ from stable In oxide and could provide new insight of catalytic CO_2 hydrogenation to methanol.

[1] C. Glass *et al.*, Comput. Phys. Commun., **175**, 713 (2006).
[2] F. Brix, and É. Gaudry, J. Vac. Sci. Technol. A, **40**, 012203 (2022).
[3] I. Batatia, *et al.*, Adv Neural Inf Process Syst, **35**, 11423 (2022).

This work was granted access to the resources of IDRIS and TGCC (allocation 99642) attributed by GENCI. Resources were also provided by the EXPLOR center hosted by the University de Lorraine (project 2017M4XXX0108).

Thermal transport measurement in Nafion thin films: the 3-omega method

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Understanding the thermal transport properties of Nafion, a perfluorosulfonic acid polymer, is essential for optimizing its use in proton exchange membrane fuel cells. In this study, we apply the 3-omega method to measure the effective thermal conductivity of Nafion thin films deposited on a soda-lime glass substrate, with measurements performed from room temperature to 95°C.

The 3-omega method allows for precise thermal measurement by using a silver metal strip heater as both the heater and sensor. This technique provides a detailed understanding of the film's thermal properties by analyzing the temperature response as a function of frequency. Initial measurements focus on the effective thermal conductivity of the combined film-substrate system, with the goal of extracting the intrinsic thermal conductivity of Nafion.

This work not only demonstrates the application of the 3-omega method to thin film systems but also highlights the importance of accurate thermal transport measurements for improving material design in fuel cell technology.

Wednesday,

November 27, 2024

Correlating multiscale structural properties to magnetic characteristics of HEAs

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In the search for the materials that possess a combination of excellent magnetic softness and vanishing magnetostriction, the ferromagnetic high-entropy alloy (HEA) system $AlCoFeNiCu_x$ (x = 0.6–3.0) was investigated. An evolution of the crystal structure and chemical composition was observed with increasing Cu content by XRD and SEM EDS characterization. The phases' constitutions and their domain sizes were characterized by correlative SEM and TEM techniques.

Magnetic softness originates from the nanostructured character of the alloys that are random mixtures of the ferromagnetic Al–Co–Fe–Ni domains and nonmagnetic or weakly magnetic Cu-rich domains on the 10 nm scale, which makes the mechanism of exchange-averaging of magnetic anisotropy efficient. The magnetic softness and vanishing magnetostriction both originate from the choice of the constituent elements (magnetic Co, Fe, and Ni and nonmagnetic Al and Cu) and the multiphase composite microstructure.

Physical properties of $Ce_xNdPrSm$ (x = 0.01-1.5) medium-entropy alloys

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Rare-earth (RE)-based high-entropy alloys (HEAs) and medium entropy alloys (MEAs), particularly light-lanthanide based, remain unexplored in terms of physical properties, compared to the heavy lanthanides. Reasons are multiple, from lanthanide contraction, which can increase the effect of lattice distortion, to low oxidation resistance and corrosion, which, for this set of measurements, had little to no effect.

This presentation will mainly cover the measurements of electrical, thermal and magnetic properties of six light RE MEAs with nominal formula $Ce_xNdPrSm$ (x = 0.01, 0.1, 0.2, 0.5, 1.0 and 1.5). All four constituent elements are magnetic and have zero pair mixing enthalpies, with XRD analysis confirming single DHCP structure in all six samples. It was discovered that the influence of Ce is higher for Ce-concentrated alloys for all measured properties, to be precise, on measurements of ac and dc magnetization in lower temperature regime, where formation of spin-glass-like phase below 15 K is observed.

$CeFe_9Si_4$: Magnetism in an intermetallic compound with transition metal and rare earth atoms

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Interesting Kondo-lattice behavior was reported for the $CeNi_9Si_4$ compound [1], since the magnetic moment of the Ni atoms is zero and the magnetic lattice is composed of an exceptionally low atomic percent of magnetic Ce atoms. This contribution will present an investigation into the magnetic properties of the isostructural $CeFe_9Si_4$.

The crystal structure of our sample, which was synthesized by arc-melting and annealing, as determined by single crystal XRD agrees with the one described previously [2]. The paramagnetic $CeFe_2Si_2$ impurity phase is non-problematic while the presence of ferromagnetic Fe_3Si inclusions need to be taken into account in the analysis.

The magnetism of $CeFe_9Si_4$, which results from the interplay of the localized Ce moment magnetism with the itinerant band magnetism of Fe, was studied by measurements of magnetism, specific heat and magnetoresistance. $CeFe_9Si_4$ is a soft magnetic material with a Curie temperature of ≈ 94 K. The presence of ferromagnetic magnetic order can be understood in the context of exchange coupling of Fe and Ce. Interestingly, in magnetic specific heat and magnetoresistance we observed a shoulder deep in the ferromagnetic phase, which we speculate results from magnetoelastic effects.

[1] H. Michor, *et al*., Phys. Rev. B **67**, 224428 (2003).
[2] D. Berthebaud, *et al*., J. Alloys Compd. **442**, 104 (2007).
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High-entropy magnetism of murunskite

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The quest to understand high-temperature superconductivity (HTS) starts by identifying a parent compound that can develop metallicity and superconductivity through doping. Murunskite ($K_2FeCu_3S_4$) is such a compound, linking the cuprates and iron-pnictides families. Like them, it shows an antiferromagnetic (AF)-like phase below 97 K. Structurally, magnetic iron atoms are randomly distributed in 2D planes, while non-magnetic copper occupies the rest, resembling a high-entropy magnetic alloy. Neutron, Mössbauer, and XPS studies reveal AF order with a quarter zone wave vector. Mössbauer spectroscopy shows iron sites with Fe^{3+} or Fe^{2+} states, which merge into a third site upon cooling, signalling an orbital transition. This sequence transforms iron atoms from a disordered state to a homogeneously ordered one, while still randomly distributed, challenging the link between crystal structure and magnetic moments in insulators.

Entropy and Structure of high entropy metallic alloys

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HEA are more than simple random distribution of few metallic elements. They are also characterized by local lattice distortions which affect the ideal configuration entropy. Composition and structural flexibility give potentially high tunable ability for adapting properties. For exemple, they have revealed interesting perspectives for hydrogen storage capacity (F. Marques *et al.*, Energy Environ. Sci. 2021). Relevant characterization of complexity is always a challenge but necessary for optimization of properties, studies and analyses. As for in the theory of information (Shannon, The bell System Technical Journal, 1948), the entropy or “uncertainty” provides a unique value for characterizing complexity, as far as it is properly evaluated. Often mentionned, the ideal entopy is most likely not relevant. An approach based on structural domains distribution (probability of occurrence of given arrangement) is proposed to evaluate an entropy of complex alloys. It was used to characterize metallic glasses and demonstrated a generalized size effect on the mechanical behavior and glass transition of amorphous phases. An attempt is made to use a similar approach using dft simulation to characterize the HEA.

High entropy alloys for solid state storage of hydrogen

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Our research is focused on materials with strong potential for solid hydrogen storage applications. We are particularly interested in compounds that possess reversible hydrogen capacities within the practical range of 1-40 bar near room temperature. This pressure range is aligned with the operating conditions of the majority of industrial electrolyzers (both alkaline and proton exchange membrane) and fuel cells.

In this presentation, we will share the latest findings on the development of high-entropy alloys. Following an in-depth examination of a range of alloys, we have identified a key indicator that enables the prediction of alloy compositions with equilibrium plateaus within the desired range. In particular, we have developed Ti-V-Cr-Mn and Ti-V-Mn-Fe based MPEAs that meet these criteria. We will also be discussing the thermodynamic properties of these alloys, along with their microstructure and crystalline structure. Furthermore, the analysis of in situ neutron diffraction experiments will provide insight into the transformations occurring during hydrogen sorption processes.

Interplay of chemical disorder and local structural dislocations in superconducting high-entropy alloys

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The first superconducting HEA $Ta_{0.34}Nb_{0.33}Hf_{0.08}Zr_{0.14}Ti_{0.11}$ was discovered in 2014 [1], exhibiting conventional mechanism with strong electron-phonon coupling (λ ~1), being supported theoretically [2]. Noteworthy, superconductivity appeared to be robust against extremely high pressures, as observed in $(TaNb)_{0.67}(HfZrTi)_{0.33}$ [3, 4], the behaviours which were preliminarily interpreted from the KKR-CPA calculations [5]. In this work, we present recent results of *ab initio* study on local distortions of the crystal structure and their influence on the electronic structure, electron-phonon interaction, and superconducting parameters in the HEA $(TaNb)_{0.67}(HfZrTi)_{0.33}$[6,7]. The largest relative changes in the interatomic distances due to relaxation reach 8%, which shows the overall strong impact of structural disorder on superconductivity in this prototype high-entropy alloy. As a consequence, the total density of states at the Fermi level and the McMillan-Hopfield parameters markedly decrease, lowering the electronic contribution to the electron-phonon coupling constant λ in 20%. This feature significantly affects the superconducting temperature, which can be reduced by about 50%.

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[7] K. Jasiewicz *et al.*, in book *High-Entropy Alloy Superconductors*, eds. J. Kitagawa &Y. Mizuguchi, Springer Series Solid-State Sci., **202**, 103 (2024).

Structural and magnetocaloric properties in rare-earth free high-entropy alloys

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We present new results on the structure and properties of rare-earth free high entropy alloys (HEAs) presenting a giant magnetocaloric effect. In order to enhance the magnetocaloric effect, the compositions of the samples were designed by applying chemical substitutions to systems known to present a magnetostructural phase transition. They are derived either from the MnNiSi ternary system or from the Ni_2MnGa Heusler type of compounds. The first family of alloys undergoes a first order magnetostructural transition. The T of the transition can be chemically tuned close to room temperature. The magnetocaloric effect is evaluated from magnetic measurements using the Maxwell relation and from direct adiabatic temperature change measurements. An isothermal entropy change as large as about 40 J.kg-1.K-1 is attained at 5 T. In the Heusler-derived HEAs, the PM/FM transition occurs at 550 K but can be tuned to lower T by Cu doping.

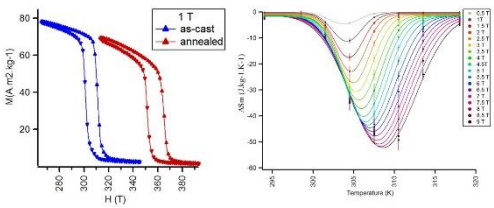

Figure 1: Thermomagnetic curves (left) and isothermal entropy change at various field in $(Fe,Mn,Ni,Co)_{66.6}(Ge,Si)_{33.3}$.

Electronic structure of compositionally complex alloys: challenges and prospects

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Compositionally complex alloys, CCA (such as the high-entropy alloys, HEA and the corresponding glassy alloys) show some excellent properties such as fatigue, irradiation and corrosion resistance as well as promising catalytic performance. However, the comprehension of their electronic structure, ES is still limited which is detrimental both for the design of CCAs and for their application. Previously we have shown that photoemission spectroscopy, PES can simply explain the evolution of properties in some CCAs with different shapes of the electronic density of states, DOS. Here, in addition to showing the correlation between the PES spectra and the evolution of intrinsic properties in selected CCAs, we also compare the theoretical DOS with the experimental one depicted from the PES spectra of these alloys. We find a considerable quantitative discrepancy between two DOSes in three HEAs for which such comparison was possible. The observed discrepancy emphasizes the importance of the experimental check of the calculated DOS in CCAs designed for specific applications [1].

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Study of lattice dynamics and electron-phonon interaction in SnTe:In and PbTe:Tl

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Resonantly doped SnTe and PbTe are well known for their exceptional thermoelectric performance, thus they have been extensively researched for decades. However, some of their properties are still not well understood. Upon doping $Sn_{1-x}In_xTe$ and $Pb_{1-x}Tl_xTe$, these compounds become superconductors with critical temperatures of few Kelvins, despite having very low carrier concentration. With so few carriers to form Cooper pairs, unconventional superconductivity of non electron-phonon origin is often proposed.

In this work, we explore electronic structure and lattice dynamics to check whether isotropic electron-phonon interaction is enough to explain superconductivity. Disordered systems were treated both with supercell approach using Quantum Espresso, VASP and Phonopy, and Korringa-Kohn-Rostoker Method with Coherent Potential Approxation. Structure relaxation lowers average phonon frequencies and enhances electron-phonon interaction around dopant atoms and neighbouring Te. Obtained electron-phonon coupling constant $\lambda \approx 0.22$ in $Sn_{31}In_1Te_{32}$ does not rule out phonon mediated pairing. Accounting for rombohedral distortion resulted in slightly higher value of λ.

Acknowledgments
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Hydrogen, oxygen, and lead adsorbates on $Al_{13}Co_4(100)$: accurate potential energy surfaces at low computational cost by machine learning and DFT-based data

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Intermetallic compounds are promising materials in numerous fields, especially those involving surface interactions, such as catalysis. A key factor to investigate their surface properties lies in adsorption energy maps, typically built using first-principles approaches. However, exploring the adsorption energy landscapes of intermetallic compounds can be cumbersome, usually requiring huge computational resources. In this work, we propose an efficient method to predict adsorption energies, based on a Machine Learning (ML) scheme fed by a few Density Functional Theory (DFT) estimates performed on *n* sites selected through the Farthest Point Sampling (FPS) process. We detail its application on the Al13Co4(100) quasicrystalline approximant surface for several atomic adsorbates (H, O, and Pb). On this specific example, our approach is shown to outperform both simple interpolation strategies and the recent ML force field MACE [arXiv.2206.07697], especially when the number *n* is small, i.e., below 36 sites. We believe that these findings and the corresponding methodology can be extended to a wide range of systems, which will motivate the discovery of novel functional materials [1].

[1] N. Boulangeot *et al.*, J. Chem. Theory Comput. **20**, 7287 (2024).

Spontaneous metal-semiconductor phase transition in atomistic simulations of liquid and amorphous Germanium

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Machine learning combined with density functional theory (DFT) computational approach dramatically boosts computational efficiency of atomistic simulations. Using this methodology, we conduct simulated cooling-heating cycles of large 512-atom sample of Germanium, and observe spontaneous first-order phase transitions between metallic and sp3 liquid/amorphous states accompanied by large change of atomic volume per Ge atom. The two undercooled states can be clearly distinguished by radial pair distributions G(R), bond angle distributions, and density of electronic states.

Electronic structure and transport properties of Fe doped γ-CuI – complex interplay of Fe impurities

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Recently, CuI has been studied as an alternative to Bi-Te based thermoelectric materials in near-room-temperature applications. Iron has been recognized as a potential power factor enhancing dopant in CuI, yet so far, no detailed studies have been reported.

Here we present results of joint theoretical and experimental investigation of Fe-doped γ-CuI. Electronic structure was obtained using fully relativistic Density Functional Theory calculations which were performed using the KKR-CPA method. Analysis of electronic dispersion relation reveals that behavior of Fe dopant depends on the presence of Cu vacancies as iron doping creates localized impurity-band-like state. Furthermore, the measurements of magnetization revealed that only a small fraction of Fe atoms was magnetic in the material. Our calculations explained that it is caused by the simultaneous presence of Cu vacancies, on-site Fe atoms and two types of interstitial Fe defects, where in the interstitial Fe becomes nonmagnetic. The presence of interstitial defects was confirmed by the Mossbauer spectroscopy. The existence of interstitial Fe atoms leads to increased power factor and reduces the lattice thermal conductivity due to higher boundary scattering and as a result enhances the ZT by about 360% when compared to the undoped CuI.

[1] S. Byeon *et al.*, J. Alloys Compd. **1002**, 175349 (2024).

Giant magnetocrystalline anisotropy energy in Fe–Co alloy under uniaxial compression: first-principles prediction

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Uniaxially strained Fe-Co alloys have recently gained attention as candidates for cost-effective rare earth-free permanent magnets due to their high magnetocrystalline anisotropy energy (MAE). We used first-principles fully relativistic calculations within the coherent potential approximation and PBE exchange-correlation potential to investigate the MAE of tetragonal Fe-Co alloys under uniaxial compression. Our findings uncovered an additional region with a high MAE. We studied the energy profiles along the broader Burgers pathway, including the transition to the fcc structure. We also enhanced the understanding of the alloy's stability by connecting the Bain and Burgers pathways [1].

[1] Marciniak et al., "Giant magnetocrystalline anisotropy energy in Fe--Co alloy under uniaxial compression: first-principles prediction." *arXiv preprint arXiv:2409.11388*, (2024).

Impact of hyperthermal oxygen on alumina surfaces investigated by molecular dynamics simulations

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Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the adsorption rate and the angular distribution of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. It is found that the angular distribution depends strongly on the surface structure and the incidence angle. A higher ratio of specular reflection is found in case of smooth surfaces and large incidence angles.

New samarium and ytterbium iron arsenides: crystal structure and physical properties

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The interest in iron arsenides of rare earth metals has been aroused by their complex magnetic properties [1]. In particular, $La_{12}Fe_{57.5}As_{41}$, $Ce_{12}Fe_{57.5}As_{41}$, $GdFe_4As_{12}$, $TbFe_4As_{12}$, and $EuFe_4As_{12}$ compounds have been reported to exhibit ferromagnetic transitions. Moreover, a ferrimagnetic transition at 29 K has been observed for the skutterudite $SmFe_4As_{12}$. Surprisingly, very little work has been carried out in the ternary systems *RE*–Fe–As, where *RE* is a rare earth metal.

In this work, we revisit Sm–Fe–As and Yb–Fe–As systems. The new ternary arsenides $REFe_5As_3$ (*RE* = Sm and Yb), which adopt the UCr_5P_3 structure type (space group $P2_1/m$), have been obtained by implementing Bi-flux method:
$SmFe_5As_3$: a = 3.8531(4), b = 7.1848(8), c = 9.7103(12) Å, β = 100.5(5)°;
$YbFe_5As_3$: a = 3.7871(9), b = 7.18491(2), c = 9.6618(8) Å, β =100.6(5)°.
The new arsenides $SmFe_5As_3$ and $YbFe_5As_3$ revealed magnetic ordering characterized by large anisotropy and magnetostriction. Magnetic phase diagrams of both materials are very rich, as a result of complex interactions between two types of magnetic ions.

[1] Villars P., Cenzual K., Eds. Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds (Release 2022/23); ASM International®: Materials Park, Ohio (USA), 2023.

Determination of the second order plastic incompatibility stresses in deformed hexagonal materials

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One of the important reasons for the formation of residual stresses in polycrystalline materials is the anisotropy of the plastic deformation process. Different slip systems activity leads to different plastic deformations of polycrystalline grains. The resulting misfit (incompatibility) between neighboring grains is the source of the second order incompatibility stresses. These stresses cannot be measured directly but can be predicted by elastoplastic deformation models. They are correlated with the nonlinearity of lattice strains $<\varepsilon(\psi,\phi)>_{\{hkl\}}$ vs. $sin^2\psi$ plots, determined experimentally. In this work the stresses in deformed titanium alloys are studied. The grazing incidence X-ray diffraction measurements carried out during an "in situ" tensile test and a novel method of interpreting the experimental data allowed us to determine the evolution of macroscopic stresses and second order stresses during elastic-plastic deformation. This work shows that second order stresses, related to microstructure of material, are generated during plastic deformation and remain in the material. It was shown that the distribution of second order stresses in the Euler space correlates with the distribution of the Schmid factor for the non-basal crystallographic systems. This confirms that these systems play a key role in generating intergranular stresses.

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Novel oxo-peroxide and oxo-superoxide phases in Ni-O binary system

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Nickel binary oxides have gained significant attention due to their potential as a foundation for new superconducting materials[1,2], as well as their importance in catalysis and photocatalysis[3,4]. The Ni-O binary system hold promise for uncovering new, functional materials and in this study, we investigate and characterize a previously unknown phase, Ni2O5. We explore the potential stabilization of Ni2O5 within crystal structures typically adopted by known pentoxides, employing Density Functional Theory (DFT). Nickel atoms are substituted for the original metal (M) atoms in the known M2O5 structures, and the suitability of these structures to accommodate Ni atoms is assessed. For this purpose, we present detailed analyses of the crystal, electronic, and phonon structures, as well as energetics. We have uncovered the potential of this system to form novel oxo-peroxide and oxo-superoxide phases, which promises interesting catalysis-related properties. Our findings contribute to a deeper understanding of structure-related properties in nickel-oxygen binary system, and the potential for new material discoveries in this system.

[1] Q. Gu, H.-H. Wen, The Innovation, **3**, 100202 (2022).
[2] D. Li, K. Lee, B.Y. Wang *et al.*, Nature, **572**, 624 (2019)
[3] M.S. N. K, J. Mater. Chem. A, **10**, 4209 (2022).
[4] M. Zhu *et al.*, Appl. Catal. B: Environ., **282**, 119561 (2021).

Acknowledgement:
Slovak Research and Development Agency, grant No. APVV-18-0168, Recovery and Resilience Plan, project no. 0910303-V04-00334, Slovak University of Technology, Grant 23-06-03-A, National Competence Centre for High Performance Computing, project code: 311070AKF2 Early State Researcher grant. of the Faculty of Materials Science and Technology of the Slovak University of Technology in Bratislava, internal number 1334

Posters

High Tc cuprates: fabrication of 2D devicess

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The phenomenon of high-temperature superconductivity in cuprates remains one of the most fascinating yet unresolved problems in solid state physics. Theoretical understanding of these materials is hindered by their complex phase diagrams and the difficulties in producing high-quality crystals, which often lead to inconsistent, and sometimes misleading, experimental data. A significant recent development showed that superconductivity in BSCCO persists with preserved normal-state properties and an undiminished critical temperature, even in samples as thin as half a unit cell. This finding enhances our understanding of superconductivity and opens the door to potential applications in quantum devices. Thin flakes of BSCCO also offer an ideal platform for transport measurements, as they are expected to have fewer defects and more uniform current flow. Although we have mastered the synthesis of high-quality BSCCO single crystals, fabricating monolayers remains highly challenging due to the material's sensitivity to environmental conditions, oxygen loss, and mechanical fragility.

Here, we present several approaches to creating monolayer BSCCO and report transport measurements on thin flakes, demonstrating that the Kohler rule, typically valid for conventional metals, holds true at optimal doping.

Surface atomic and structure of In_3Ni_2 intermetallic.

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These days, studying surface science and comprehending surface and vibrational properties is an important area of academic research. By understanding these matters relating to surfaces, it is easy to compare materials and modify or choose inexpensive materials with the same properties. The specific goal of this project is to understand the surface atomic structure of catalysis.

This sample consists of Nickel (Ni) and Indium (In) elements In_3Ni_2 intermetallic catalyst in the trigonal P-3m1 space group. In fact, there is scant information available about the sample.

This process is performed under high pressures and temperatures using Ultra-high vacuum (UHV) technology to maintain a clean sample surface and provide a good environment to avoid destroying the samples. Additionally, various surface analysis techniques attached to UHV devices are applied, such as Low Energy Electron Diffraction (LEED) to examine the symmetry of the surface and provides information on the arrangement of atoms on the surfaces. Also, scanning Tunnelling Microscopy (STM) used to recognise the three-dimensional profile of the surface structure and chemical components.

This project will work in the lab located at the Surface Science Research Centre at the University of Liverpool and Institut Jean Lamour.

Magnetotransport properties of selected high entropy alloys

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This research is focused on metallic glass ribbons from three alloy systems: $(TiZrNbNi)_{1-x}Cu_x$, $(TiZrNbCu)_{1-x}Ni_x$, and $(TiZrNbCu)_{1-x}Co_x$, spanning a broad composition range. In addition, measurements were conducted on an amorphous thin film of TiZrNbCuNi, which was deposited on a SrLaAlO4 substrate using a pulsed laser deposition (PLD) system. The results of resistivity, Hall effect, magnetoresistance, and superconductivity measurements largely agreewith those reported in previous investigations on related binary and ternary amorphous alloys. We identified a novel model of two parallel conducting channels in 20–200 K range, composed of a metal-like and a variable range hopping (VRH)-like channel, that describes the temperature variation of resistivity observed in our and other experiments. A mechanism for the origin of these two conductance channels is discussed in more details.

Synthesis and structural analysis of ZnMgEr P-type quasicrystals

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Up to now, only one atomic strucutre was successfully solved in the group of Bergman type quasicrystals which is $Zn_{70}Mg_{20}Tm_{10}$ P-type phase. In this contribution, we synthesised new samples in ZnMgEr familiy by self-flux method. Selected crystals were measured by a single crystal X-ray diffraction resulting in approximately 2500 peaks ($|F|<u(|F|)$). The finalk model achieved R-factor around 14% (Figure 1.) with less then 350 parameters. The model was significantly constrained comparing to ZnMgTm resulting in the reduction of parameter number. The future work will be dedicated to improve the quality of the diffractiondata

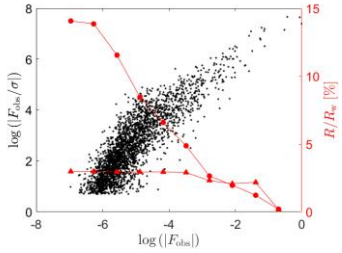

Figure 1. The aggreement between experimental and calculated diffraction amplitudes.

Acknowledgement: The work was supported by the grant 2022/47/I/ST3/00340 from the Polish National Science Centre

Theoretical investigation of novel palladium suboxide Pd_2O

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Palladium and its compounds play a significant technological role in industries like automotive, pharmaceuticals, and agriculture, acting as essential catalysts. Increasingly, palladium oxides are also being recognized for their catalytic properties [1], although they remain poorly understood. Currently, only two palladium oxides, PdO [2] and PdO_2 [3], are recognized. In this study, we focus on the theoretical exploration and prediction of the crystal structure of the poorly characterized Pd_2O. This suboxide has been identified only in very thin palladium films, with a proposed cuprite structure (space group *P*n-3m) [4], but has not been further analyzed, leaving its properties largely unknown. To better understand Pd_2O, we have calculated its crystal, electronic, and phonon structure based on the reported cubic phase, and evaluated its thermodynamic stability using Density Functional Theory. Additionally, by applying evolutionary algorithms for crystal structure prediction, we have identified new possible polymorphs of Pd_2O. Our results indicate that Pd_2O can exist in multiple modifications of the cuprite type structure. These modifications hold promise for the possibility of desirable tuning of semiconducting and metallic properties of this material.

Acknowledgement*: Slovak Research and Development Agency, grant No. APVV-18-0168, Recovery and Resilience Plan, project no. 0910303-V04-00334, Slovak University of Technology, Grant 23-06-03-A, National Competence Centre for High Performance Computing, project code: 311070AKF2*

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Single crystals of Nd-Fe-B permanent magnets and UHV surface investigation of their surface structure.

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Rare-earth-element (REE) permanent magnets based on Nd–Fe–B are vital for use in electric vehicles and wind turbines, making then central to Europe's green-energy future. The European project GREENE will focus on a redesign of Nd-Fe-B magnets as an advanced material where the Nd in the grain boundary is replaced by a specific designed interface material in order to address the problem of translating the under-used intrinsic properties of the hard-magnetic $Nd_2Fe_{14}B$ phase into better extrinsic properties of the magnet. The poster will present a summary of the results obtained so far on the growth of $Nd_2Fe_{14}B$ single crystals and UHV surface investigation of their surface structure.

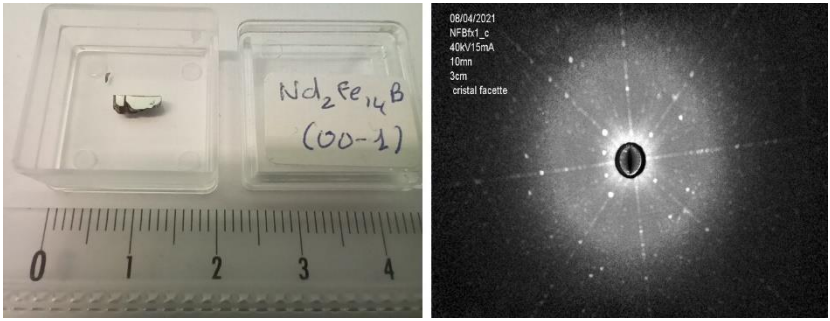

Figure: Single crystal of the $Nd_2Fe_{14}B$ obtained by a flux method and corresponding Laue diffraction pattern.

Investigation of excitation-induced non-thermal effects in semiconductors, metals and alloys

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Excitation-induced non-thermal melting in silicon, as well as bond-hardening in gold following strong laser irradiation with short pulse durations have been known for several years. Furthermore, several traces of excitation-induced solid-solid phase transitions have been noticed in a variety of materials.

Here, we present several approaches to identify and quantify excitation-induced effects changing the bond strength and inducing phase transitions systematically in several semiconductors, metals and alloys obtained from DFT calculations depending on the degree of excitation. These calculations are in line with previous investigations and provide new insights into the change of the bond strength and the induced phase transitions following strong laser excitation. We also report recent advances in the inclusion of such effects in large-scale simulations.

XRD/FIB/SEM characterization of the CexPrNdSm high-entropy alloys

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Here we present the rare kind of the HEAs composed of the light lanthanide series. We investigated the Ce-Pr-Nd-Sm HEAs for a range of compositions $Ce_xPrNdSm$, where the Ce concentration x is systematically varied from Ce-diluted composition (x = 0.01) to Ce-concentrated compositions (x = 0.1, 0.2, 0.5, 1.0 and 1.5).

XRD spectra of the $Ce_xPrNdSm$ alloys all demonstrate dhcp (double hexagonal close packed) structure. The dhcp structure shows many diffraction peaks that are common with the hcp structure (hexagonal close packed) for the ratio of the dhcp and hcp unit-cell parameter c 2:1.

Due to the easy oxidation of the rare earths elements, the samples had to be treated and prepared for SEM electron microscopy in vacuum. It was done in FIB with a Ga ion beam. The further SEM investigations revealed homogeneous composition on the micrometer scale of all samples.

Physical properties of supersilent $(GaNi)_xCoCrFe$ high-entropy alloys

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In a search of high-entropy alloys (HEAs) with functional physical properties emerging from their multi-scale structure, we have studied the $(GaNi)_xCoCrFe$ (x = 0.4–1.6) system. We conducted a comprehensive characterization of the structure, microstructure, nanostructure, and chemical composition of the individual phases within the multi-phase alloys, and examined their magnetic, magnetostrictive, and electrical properties. Our findings indicate that these alloys are ferromagnetic and exhibit a unique combination of magnetic softness and negligible magnetostriction, identifying them as energy-efficient "supersilent" materials (inaudible to the human ear) for alternating-current (AC) electromagnetic applications in the audio-frequency range.

The alloys develop a two-phase structure consisting of a face-centered cubic (fcc) and a body-centered cubic (bcc) phase, with the fraction of the fcc phase decreasing as the $(GaNi)_x$ content increases, while the bcc fraction correspondingly increases. In the alloy with the highest x = 1.6 content, the fcc phase disappears entirely, and a minor $D0_3$ phase forms alongside the bcc phase. The ferromagnetism in these alloys is attributed to the highly nanostructured bcc phase, with Curie temperatures (T_C) ranging from 750 to 700 K, depending on x. The fcc phase, on the other hand, is not nanostructured, and remains paramagnetic at room temperature, while it undergoes a spin glass transition at $T_f \approx 6.4$ K.

Both the magnetic softness and the negligible magnetostriction observed in these alloys are nanomagnetic phenomena. The magnetic and magnetostriction characteristics of the alloys with x = 1.3 and 1.6 render them particularly suitable for supersilent AC applications at low frequencies.

Single-grain re-engineered Nd-Fe-B permanent magnets.

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The GREENE project funded by the European Commission addresses one of the Europe's Grand Societal Challenges, aligned with the European Green Deal and the recently released Green Deal Industrial Plan for the Net-Zero Age, which alongside the Circular Economy Action Plan, sets the framework for the transformation of the EU's industry. Rare-earth-element (REE) permanent magnets based on Nd–Fe–B are vital for use in electric vehicles and wind turbines, making then central to Europe's green-energy future. These magnets have outstanding properties, but they are not without their weaknesses. There is, of course, the well-known dependence on imports from China, on which Europe is presently totally dependent. However, here, in line with the scope of the Resilient value chains 2023 call, GREENE will focus on a redesign of Nd-Fe-B magnets as an advanced material where the Nd in the grain boundary is replaced. At the same time, GREENE will address the problem of translating the under-used intrinsic properties of the hard-magnetic $Nd_2Fe_{14}B$ phase into better extrinsic properties of the magnet. The poster will present a summary of the objectives of this project.

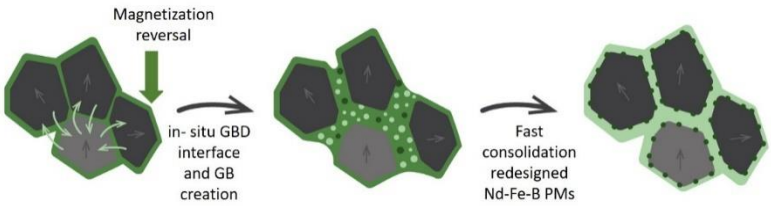

Figure: Schematic of the methodology adopted in the single-grain re-engineered Nd-Fe-B permanent magnets project.

Magnetic softness and vanishing magnetostriction in high-entropy alloys $(GaNi)_xCoCrFe$ (x = 0.4–1.6)

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Searching for high-entropy alloys (HEAs) with functional physical properties arising from their multi-scale structure, we investigated the $(GaNi)_xCoCrFe$ (x = 0.4–1.6) system. We characterized the alloys' structure, microstructure, nanostructure, and chemical composition, as well as their magnetic, magnetostrictive, and electrical properties. The alloys exhibit ferromagnetism with a distinctive combination of magnetic softness and vanishing magnetostriction, making them ideal "supersilent" materials for energy-efficient alternating-current (AC) electromagnetic applications in the audio-frequency range. The two-phase structure consists of a face-centered cubic (fcc) and body-centered cubic (bcc) phase, with the fcc fraction decreasing and bcc fraction increasing as $(GaNi)_x$ content rises. At x = 1.6, the fcc phase is absent, and a minor $D0_3$ phase emerges alongside the bcc phase. Ferromagnetism originates from the nanostructured bcc phase, with Curie temperatures between 750–700 K, while the fcc phase is paramagnetic and undergoes a spin glass transition at $T_f \approx 6.4$ K. The alloys' magnetic softness and vanishing magnetostriction, both nanomagnetic phenomena, make the x = 1.3 and 1.6 compositions suitable for low-frequency supersilent AC applications.

Temperature dependent electrical resistivity measurement of Mn_2P under high pressure

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Mn_2P features a non-centrosymmetric hexagonal structure (space group: $P\bar{6}2m$) with two distinct Mn sites and exhibits antiferromagnetic ordering below a Néel temperature (T_N) of ~103 K [1]. Despite extensive research [1, 2], the magnetic structure of Mn_2P remains unclear, and inconsistent electrical resistivity curves as a function of temperature depending on crystal morphology were reported [3]. These conflicting results underscore the need for further investigation using high-quality single crystals to uncover the intrinsic magnetic and electronic properties of Mn_2P. In present study, we optimized method for growing single crystals of Mn_2P using the Sn-flux method. The chemical composition and crystal structure were analyzed by energy dispersive X-ray spectroscopy and powder X-ray diffraction, confirming the composition as Mn_2P. We also measured the magnetic susceptibility and its field dependence on the grown single crystals. The results indicate an antiferromagnetic transition at T_N = 104 K and a spin-reorientation transition while applying the field along the *c*-axis. The grown crystals attain lower residual resistivity than the earlier studies [3, 4]. With increasing pressure, up to 6 GPa, T_N rises, then tends to decrease under higher pressure, hinting at a potential quantum critical point. The details of the electrical resistivity measurement under pressure will be discussed in the poster presentation.

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[4] S. Na *et al.*, CPL. **37**, 087301 (2020).

Single crystal synthesis of doped murunskite

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Recently, we successfully synthesized high-quality single crystals of murunskite ($K_2FeCu_3S_4$) for the first time [1]. This compound serves as a bridge between cuprates and iron-pnictides—the only two known families of high-Tc superconductors. Like the parent compounds of cuprates, murunskite is an insulator [1], similarly exhibiting antiferromagnetic-like ordering at 100 K [2]. However, it shares the same structure as the metallic 122 family of iron-pnictides. This combination suggests exciting potential for exploration through doping strategies.

The aim of this research is to develop and apply effective substitution and doping techniques at both ligand and metal sites, using elements such as As, Se, Zn, Co, and Ni. The resulting single crystals are thoroughly characterized through various experimental methods, including X-ray spectroscopy, magnetic susceptibility, and resistivity measurements.

[1] D. Tolj, *et al.*, Applied Materials Today, **24**, 101096 (2021).
[2] D. Tolj, *et al.*, *arXiv:2406.17108* (2024).

Characterization of lightweight TiAlSc multi-principal element alloy

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Traditional lightweight metal materials have certain limitations. For example, aluminium alloys have relatively low strength, magnesium alloys exhibit poor plasticity and corrosion resistance at room temperature and are difficult to process, and titanium alloys tend to be expensive. As a result, the development of lightweight metal materials for industrial applications is one of the most challenging research areas today. In our study, a new lightweight TiAlSc alloy was prepared and investigated. The alloy has a density of approximately 3.5 g/cm³. The microstructure characterization and selected mechanical properties of the prepared alloy will be presented and discussed.

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Role of the functional group effect in tailoring rare supramolecular copper(II) magnetic architectures

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In crystal engineering, the art of tailoring novel crystal materials involves knowledge of the electrostatics, sterics, and topologies of intermolecular interactions between self-assemblies of small building blocks. Apart from using this knowledge as an engineering tool in building supramolecular architectures, these factors also play a central role in molecular magnetism, either as mediators of magnetic exchange coupling or as structural features that significantly influence existing magnetic pathways. However, understanding the key effects of functional groups on magnetic exchange interactions, particularly in metal-organic systems has received much less attention. To elucidate magneto-structural relationships considering electron-withdrawing functional groups (EWG), electron-donating functional groups (EDG), and the effects of inductive and resonance interactions, we opted to tailor a series of one-dimensional halide coordination polymers of copper(II) with halogen derivatives of pyridine.

For all obtained coordination compounds ($[CuX_2(3\text{-}Rpy)_2]_n$, where X=Cl, Br; R=Cl, Br, I), we measured the temperature dependence of magnetization $M(T)$ using a SQUID magnetometer over the range of 2–300 K. In accordance with the crystal structure, we applied the Bonner–Fischer approach to model the entire $M(T)$ curves for all obtained compounds, using a spin chain of antiferromagnetically interacting neighboring Cu^{2+} ions along structural chains. We observed the impact of the counterion and the nature of key functional groups on the superexchange interaction J.

Synthesis and Characterization of Magnetic and Transport Properties in Intercalated TMDs

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Transition metal dichalcogenides (TMDs) are layered materials that exhibit intriguing phases like charge density waves (CDW) and superconductivity. The layered structure allows for intercalation with first-row transition metals, which can suppress CDW and superconducting ground states while enabling various magnetic orderings. We synthesized high-quality single crystals of Ni_xNbS_2 ($0.01 < x < 0.6$) and stoichiometric $Co_{1/3}TaS_2$. In the case of Ni_xNbS_2We investigated the suppression of the parent compound SC state at low intercalations and the impact of disorder on the magnetic ground state. In $Co_{1/3}TaS_2$ as well as $Ni_{1/3}NbS_2$, we also conducted ARPES to investigate the effect of intercalation on the electronic structure near the Fermi level. Ongoing magneto-transport experiments and studies on the impact of uniaxial pressure aim to provide a more comprehensive understanding of these materials and their electronic structures.

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Thermal expansion of CoFeNiCu-based multi-principal element alloys

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In this contribution, the effect of copper content on the thermal expansion of CoFeNiCu-based multi-principal element alloys was investigated over a temperature range of -50°C to 900°C. The CoFeNi alloy consists of a single face-centered cubic phase (FCC-1). As copper is added and its concentration increases relative to the CoFeNi elements, a Cu-rich secondary face-centered cubic phase (FCC-2) gradually forms. The theoretical values of the coefficient of thermal expansion (CTE) can be described by combining the Debye–Grüneisen relation with the Arrhenius equation for vacancy formation. In this study, both the experimental and theoretical dependence of CTE on temperature were examined. Deviations between the experimental and theoretical CTE values will be presented and discussed.

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Growth and characterization of CoCrFeNi on $LaAlO_3$ substrates

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High-entropy alloys (HEAs) are a class of materials composed of four or more principal elements in near-equimolar proportions. This composition is expected to favour the formation of single-phase solid solutions. Initially reported and investigated by Cantor *et al.* [1] and Yeh *et al.* [2] in 2004, HEAs have gained significant interest due to their unique properties. Although engineering and materials research has progressed, surface science studies remain scarce, potentially due to the lack of high-quality samples. In an effort to fill this gap, Schwarz *et al.* recently demonstrated the crystalline growth of CoCrFeNi on MgO(100) by DC-magnetron sputtering [3]. Nevertheless, these films exhibit some defects due to the large lattice mismatch between the layer and the substrate. To improve on film quality, we investigate the use of $LaAlO_3$ (LAO) as a substrate, which offers a lattice constant much closer to that of CoCrFeNi and enables the growth on all low index surfaces. Utilizing the techniques of X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and angle-resolved photoemission spectroscopy (ARPES), we demonstrate the successful growth of CoCrFeNi on all low-index surfaces of LAO.

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[2] Yeh *et al.*, Adv. Eng. Mater., **6**, 299 (2004).
[3] Schwarz *et al.*, Adv. Mater., **35**, 2301526 (2023).

Quantum oscillations in Sn-doped BST2S topological insulator

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Topological insulators (TI) have recently gained a lot of attention due to interesting properties attributed to surface states (SS), which appear because of spin-orbit coupling-assisted band inversion. Although the bulk remains insulating, surface bands cross each other and remain topologically protected inside the band gap. Moreover, SS are spin–momentum locked, making TI prominent for spintronic devices. The challenge is to experimentally realize systems where bulk is insulating, Fermi level position is inside the gap, spin-orbit coupling is strong enough, and high-quality single crystal synthesis is possible.

In this work, Sn-doped BST2S single crystals have been synthesized using the modified Bridgman technique. Measurements of resistivity show the contribution of bulk at higher temperatures and dominance of surface states below 150 K. Magnetoresistance measurements have SdH oscillations at 2 K related to metallic SS. The system has transitioned from p-type carriers at higher temperatures to n-type carriers below 150 K acquired from Hall measurements. Fermi level position can be estimated by Arrhenius plot of the resistivity showing Fermi level is at 130 meV below the conducting band. Fermi level has been measured by ARPES and Seebeck coefficient, both corroborating the Fermi level position.

Analysis of the frequencies of magnetic moment measurements reveals an unusual evolution with temperature that cannot be explained by the Sommerfeld chemical potential shift (due to higher temperatures) and the topological contribution for the linear dispersing bands.

The study of electronic transport properties of transition metal dichalcogenides under uniaxial pressure using a piezo-driven stress cell

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Transition metal dichalcogenides (TMDs) are examples of layered materials that have been intensively studied in recent years. These particular systems are often a source of interesting phases, such as charge density waves (CDW) or superconductivity. Additionally, electronic, magnetic, and elastic properties can be finely tuned by the intercalation of magnetic ions. Furthermore, the ground states can be influenced by exposing samples to external stimuli, such as high pressure.

In this study, we investigate the electronic transport properties of some host and intercalated TMDs under uniaxial pressure. We have used the Razorbill piezo-driven stress cell (FC100 model) in two modes – tension and compression. The working principle of the cell will be described, and we will present the effect of uniaxial stress on the change in phase transition behaviors.

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Institute of Physics – From participation in the European Network of Excellence, NoE CMA to the partner institution of the European Integrated Centre (EC-MetAC)

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On the occasion of the 15th anniversary of the European Integrated Centre for the Development of New Metallic Alloys and Compounds (EC-MetAC, hereinafter referred to as "the Centre"), in which the Institute of Physics has actively participated since its inception in late 2009, we would like to highlight the sginificant contributions made by the Institute of Physics in cooperation with the Centre members, resulting in numerous published scientific papers. Furthermore, the Institute has been instrumental in promoting the education and development of young scientists, fostering the creation of master's and doctoral theses within this specialized field.

The Institute of Physics has actively encouraged research in this area among scientists across Croatian academic and research institutions. This ongoing support has facilitated partnerships with key institutions, including the Faculty of Science in Split (2018) and the Department of Physics, Faculty of Science, University of Zagreb (2022), which is co-organizing the ECMetAC Days 2024.

Looking forward, we continue to pursue new research avenues within the Centre, particularly through collaboration with the recently established Laboratory for Synthesis, led by Professor Neven Barišić at the Department of Physics, University of Zagreb.

Magnetotransport in crystal rutile and anatase

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It is proposed that anatase and rutile, two mineral forms of titanium dioxide TiO_2, are systems where large (anatase) and small polaron excitations (rutile) occur. Polaron is a quasiparticle which consists of a free electron and an accompanying phonon cloud. It is being intensively investigated because of its still partially unknown effect on transport properties [1]. Our results of temperature-dependent resistivity of anatase and rutile crystals show an activated behavior between 5 K and 30 K, which is considered to originate from polaron contribution. The magnetic field dependence of the activation energy increases linearly with the magnetic field, which can be explained by the discretization of the electron energy into Landau levels and their dependence on the magnetic field. The magnetoresistance data at low temperatures show an Efros–Shklovskii type of conduction.

[1] C. Franchini *et al.*, Nat. Rev. Mater. **6**, 560 (2021).

Spin-glass phase in Zn-Mg-*RE* (*RE* = Er, Tm) quasicrystals

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This contribution will present a preliminary study on the magnetism in primitive (P) and face-centered (F) phases of Zn-Mg-Tm and Zn-Mg-Er icosahedral quasicrystals. Single crystals of ~1 mm size grown by the self-flux method were used in all the experiments. The measurements of the temperature-dependent zfc and fc magnetization show paramagnetic behaviour down to ~1 K for all samples. Below about 1 K, splitting between M_{fc} and M_{zfc} occurs, M_{zfc} exhibits a cusp, and a peak appears in the specific heat that broadens and shifts in the external field – all characteristic of a transition to a spin-glass phase.

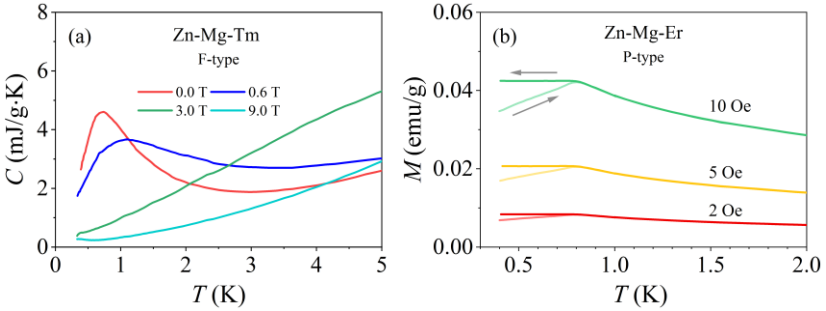

Figure 1: (a) Specific heat below 5 K in the magnetic field range of 0−9 T. (b) Temperature-dependent zfc and fc magnetization of Zn-Mg-Er.

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