European CMetAC

ECMetAC Newsletter No. 15

August 2025

Dear colleagues of the ECMetAC network,

Ronan McGrath served as Secretary General since the start of the network – thank you very much Ronan! – and is now followed by Hem Raj Sharma from University of Liverpool.

Staying with Liverpool, the series on presentation of the partner labs is continued in this issue and the facilities in Liverpool are presented. If you are interested in presenting your lab in the newsletter, please get in contact with Julian Ledieu

This summer was one of the hottest in the records – read upon some of the research ongoing in the network to allow for the transition towards a sustainable energy infrastructure in this newsletter.

Following our splendid meeting in Zagreb in November 2024 the next ECMetAC Days will take place from 24th to 27th of November 2025 at Empa in Dübendorf, Switzerland. Preparations are running full steam, **registration and abstract submission will close on the 9th of September 2025**. We are looking forward to Welcoming all of you at our yearly meeting in Dübendorf!

We wish you all a good summer, interesting research results and the quantum of luck necessary in your experiments and calculations!

Best wishes,

Julian Ledieu, Hem Raj Sharma,
Marc Armbrüster, Jean-Pierre Celis
and Émilie Gaudry

Our Network is Growing – New Partner!

The Faculty of Materials Science and Technology, located in Trnava, is the latest member of ECMetAC and the youngest faculty of the Slovak University of Technology in Bratislava, one of Slovakia's leading research universities.

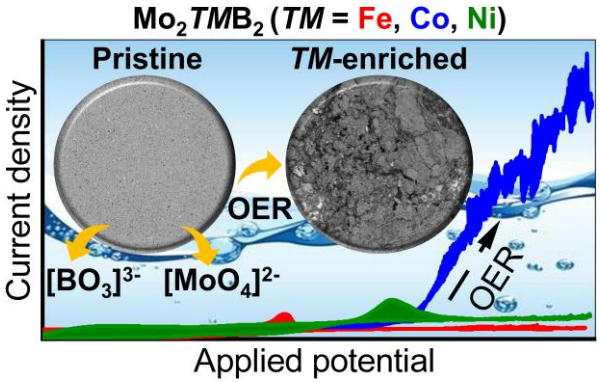
The faculty focuses on education and research in materials engineering, advanced manufacturing technologies, automation, management, and safety engineering. Its modern campus includes the first university science park in Slovakia and over 30 specialised laboratories.

Research in advanced materials is one of the faculty's core strengths. Key areas include surface engineering and thin film deposition, ion beam analysis and modification of materials, laser processing, and the development of nanostructured and high-performance alloys, as well as the preparation of new metallic systems with tailored mechanical, chemical, and physical properties. Complementing experimental work, the faculty also conducts computational materials science using ab initio methods, particularly density functional theory (DFT), to study the structure, stability, and thermodynamics of advanced alloys and compounds, providing insights that accelerate the development of innovative materials.

The faculty maintains strong links with industry and participates in international projects, ensuring that research outcomes are both scientifically significant and industrially relevant.

News from the Research and Activity Domains (RADs)

Chemical Behavior of Mo2TMB2 (TM = Fe, Co, Ni) upon the Oxygen Evolution Reaction (OER)



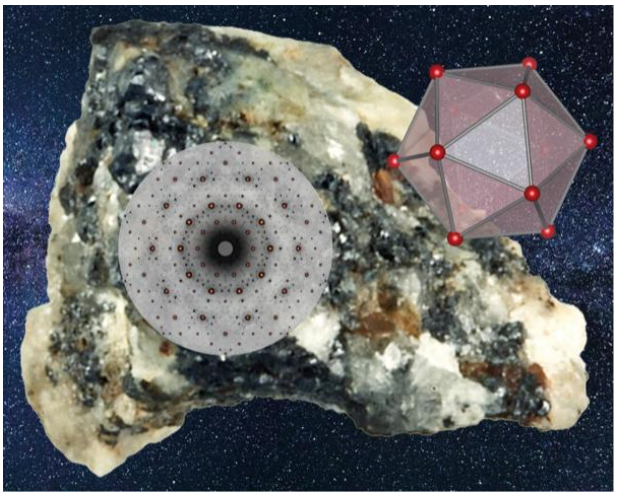
The study sheds light on how intermetallic compounds Mo_2TMB_2 (*TM* = Fe, Co, Ni) behave under the oxygen evolution reaction (OER) – a challenging half-reaction of water electrolysis. The combined electrochemical measurements, detailed bulk- and surface-sensitive material characterization revealed that **Mo_2FeB_2** surface oxidation begins even upon air exposure, forming MoO_3, Fe_2O_3, and B_2O_3. Under OER conditions, this process deepens, leading to the formation of a poorly conductive Fe_2O_3 layer and a loss of OER activity. **Mo_2NiB_2** possesses different behavior depending on applied conditions, but consistently undergoes significant Mo and B dissolution, resulting in continuous degradation during anodic polarization. In contrast, **Mo_2CoB_2** stands out for its high OER activity. The dynamic surface modification with formation of Co_3O_4 and $Co(OH)_2$ enables the OER to start at significantly lower overpotentials than elemental cobalt. These findings clearly reveal that insight into the chemical behavior of catalyst materials under reaction conditions is necessary step for interpretation of their catalytic performance.

F. Aras, U. Burkhardt, A. Ormeci, H. Borrmann, S.G. Altendorf, Yu. Grin, I. Antonyshyn

ACS Materials Au 5, **2025**, 718.

https://doi.org/10.1021/acsmaterialsau.5c00035

High resolution X-ray study of the icosahedrite, an icosahedral AlCuFe quasicrystal from a meteorite



Icosahedrite, natural icosahedral $Al_{63}Cu_{24}Fe_{13}$, was discovered in a meteorite about 15 years ago. We have carried out a high-resolution X-ray diffraction study on a sample of this meteoritic mineral at the ESRF. The diffraction pattern turns out to be identical to an intermediate phase observed in synthetic i-AlCuFe when transforming from the quasicrystalline state to a periodic rhombohedral phase. This particular natural $Al_{63}Cu_{24}Fe_{13}$ grain is an icosahedral quasicrystal on which is superimposed a modulation by six cosine waves propagating along the 5-fold axes, with a wavelength of about 20 nm and a polarization in the phason/perpendicular space. By examining the thermodynamic conditions for producing this modulated icosahedral phase at high pressure in the laboratory, we may gain insights on the formation process of the Khatyrka meteorite.

H. Takakura, K. Mizunuma, T. Yamada, A. Bosak, F. Formisano, L. Paolasini, M. de Boissieu, P.J. Steinhardt, L. Bindi

IUCrJ 12, **2025**, 435.

https://doi.org/10.1107/S2052252525004130

Partner News

Graduation

Oscar Shedwick graduated with his PhD from the University of Liverpool in May 2025. His thesis, entitled Surface Chemical Composition, Atomic Structure and Oxidation of the Ga_3Ni_2 Intermetallic Catalyst, involved studying the surface symmetry, chemical composition, and structure of an intermetallic compound with potential applications as an industrial catalyst for converting CO_2 into methanol at atmospheric pressure. This was achieved using a wide range of analytical techniques, with a primary focus on scanning tunnelling microscopy (STM) and X-ray photoelectron spectroscopy (XPS), all carried out under an ultrahigh vacuum (UHV) environment.

His work has been presented at several ECMetAC events over the past four years, and he had the opportunity to work with Dr Julian Ledieu, Dr Vincent Fournée, and Dr Wilfried Bajoun Mbajoun for two weeks at L'Institut Jean Lamour (IJL) in Nancy, under the ECMetAC Youth Exchange scheme. Oscar was co-supervised by Dr Hem Raj Sharma and Prof Ronan McGrath (Surface Science Research Centre).

Young Scientists in the Network

My name is Mathis Couderc, a second-year engineering student and research assistant at the Institut Jean Lamour, where I have the opportunity to be supervised by E. Gaudry, J. Ledieu and L. Dezerald, on a research project focused on the adsorption of the C_{60} molecule on the $Al_{13}Fe_4$(010) substrate. The objective of this work is to computationally model the relaxed adsorption positions of C_{60} and to simulate scanning tunneling microscopy (STM) images in order to compare them with experimental observations.

This is a fascinating project that I have been working on for a year now, alongside my engineering studies. It has allowed me to discover the world of research and to deepen my understanding of scientific concepts I had never encountered before, such as density functional theory and adsorption energy calculations. I started with no specific background in the field, only a desire to learn — and this project has provided a truly valuable learning experience.

Although I do not intend to pursue a career in research, my time at the Institut Jean Lamour has been incredibly enriching. It has given me new skills, a more rigorous approach to work, and a broader understanding of what it means to be an engineer. In short, I believe research is an excellent training ground for becoming a well-rounded engineer!

Partner Introduction

Surface and Nanoscale Properties of Quasicrystals and Intermetallic Compounds

1. Scope of Work

The research group at the University of Liverpool, comprising Emeritus Prof. Ronan McGrath, Dr. Hem Raj Sharma, Dr. Sam Coates, and their PhD students, focuses on the characterisation of surface properties of novel materials, with interests of both fundamental research and applications. These materials include quasicrystals - solids that never repeat periodically yet exhibit long-range order, and Intermetallic catalysts - compounds with precisely ordered atomic structures that can exhibit unique catalytic properties.

2. Research Topics

Surface properties of quasicrystals

We utilise a variety of experimental surface science techniques to investigate the surface properties of quasicrystals and their periodic counterparts (approximants). Our focus includes surface atomic structure, electronic

structure, chemical composition, surface diffusion, adsorption, and oxidation behaviour. These studies are motivated both by fundamental science and by surface-driven applications such as corrosion resistance and catalysis.

Ultrathin films with novel structures
We fabricate ultrathin films of molecules and metallic elements with unique structures, using quasicrystals as substrates. Examples include quasicrystalline molecular films [1] and multilayer quasicrystalline thin films composed of single elements. Our aim is to understand the relationship between quasiperiodic order and physical properties, using these structures as model systems, as well as the factors that influence ordering processes during growth.

Multiscale quasiperiodic architectures
We extend the study of atomic-scale quasicrystals to large-scale quasiperiodic architectures fabricated via nanolithography and 3D printing. These artificial structures allow us to investigate fundamental properties, such as quasicrystalline artificial spin ice - arrays of single-domain nanomagnets arranged in a quasiperiodic tiling and functional properties in photonics and mechanics.

Theoretical studies of quasiperiodic structures
We explore the mathematical foundations of quasiperiodic structures and their applications in magnetism, waveguide arrays, advanced mechanical materials, and beyond. This includes but is not limited to the generation and characterisation of new quasiperiodic tilings and computational studies (e.g., Monte Carlo simulations) of their physical properties [2].

Intermetallic catalysts
Intermetallic compounds are promising low-cost, environmentally friendly alternatives to noble-metal catalysts due to their tunable chemical composition and electronic structure. We investigate their surface properties and adsorption behaviour under ultrahigh vacuum to gain insight into the fundamental mechanisms governing catalytic reactions, with the aim of optimising catalytic performance. This work is carried out in collaboration with ECMetAC partners.

3. Experimental Techniques
Our in-house facilities include UHV-based surface science equipment such as Omicron variable-temperature scanning tunnelling microscopy (VT-STM). Low-energy electron diffraction (LEED), and Facilities for ultrathin film growth. The University of Liverpool also provides shared facilities, including Low-energy ion scattering (LEIS) for elemental analysis of the outermost atomic layer, additional capabilities may be available through collaboration, such as thermal scanning probe lithography (t-SPL) - a nanoscale lithography technique, additive manufacturing methods, including direct ink writing (DIW) and stereolithography (SLA).

UHV chamber equipped with an Omicron variable-temperature STM, LEED, and a thin-film growth facility.

Contact
For further inquiries, please contact Dr. Hem Raj Sharma: H.R.Sharma@liverpool.ac.uk or visit https://www.liverpool.ac.uk/people/hem-sharma

References
[1] Coates et al., *A molecular overlayer with the Fibonacci square grid structure*, Nature Communications 9, 3435 (2018).
[2] Coates, *Designing aperiodic to periodic interfaces*, J. Phys. A: Math. Theor. 58, 235001 (2025).
[3] Alfahad et al., *Atomic Structure, Chemical Composition, and Oxidation Behaviour of the (001) Surface of Ni_2In_3 Intermetallic Catalyst*, Physical Review Materials 9, 035801 (2025).

Event Reports

16th International Conference on Quasicrystals (ICQ16)

Nancy, France, June 2025

The 16th International Conference on Quasicrystals (ICQ16) was held in Nancy, France, from June 22nd to 27th, 2025. This is one of the series following the 1st workshop in Les Houches, France, the 2nd in Beijing, China, the 3rd Meeting in Vista-Hermosa, Mexico, the 4th Conference in St. Louis, USA, the 5th in Avignon, France, the 6th in Tokyo, Japan, the 7th in Stuttgart, Germany, the 8th in Bangalore, India, the 9th in Ames, USA, the 10th in Zürich, Switzerland, the 11th in Sapporo, Japan, the 12th in Cracow, Poland, the 13th in Kathmandu, Nepal, the 14th in Kranjska Gora, Slovenia, the 15th in Tel-Aviv, Israel.

ICQ16 covered a wide range of topics on quasicrystals, including:

- Formation, growth and phase stability
- Structure and modeling
- Mathematics of quasiperiodic and aperiodic structures
- Physical properties: transport, magnetic, dynamical, mechanical etc.
- Surfaces and overlayers, reactivity, catalysis
- Applications

The conference (https://icq16-conference.com/) offered an excellent opportunity for researchers working on **quasicrystals** and related topics to discuss on **emerging research**, exchange ideas, establish dialogues and encourage active collaborations with other research groups, hence promoting **material science** and **engineering**. This conference brought together the best scientists in the world to making a major contribution in the recent developments in this field.

ICQ16 was attended by 85 participants from 18 countries. There were 15 scientific sessions, 15 invited talks, 37 contributed talks as well as 2 poster sessions. The conference was truly interdisciplinary - comprising theoretical and experimental physicists, mathematicians, chemists and materials scientists.

The 2025 Jean-Marie Dubois Award for Excellence in Quasicrystal Research was attributed to **Ryuji Tamura**, Professor at Tokyo University of Science, Japan. The Jean-Marie Dubois Award was established to recognize important, sustained research on any aspect of quasicrystals in the last 10-year period preceding the award. Prof. **Ryuji Tamura received this award** in recognition of his outstanding achievements in establishing the long-range magnetic orderings in periodic approximants and quasicrystals, with the recent discovery of ferromagnetic and antiferromagnetic orders in Tsai-type icosahedral quasicrystals.

In addition, the support from the International Union of Crystallography (IUCr) permitted seven travel grants to be attributed to young scientists. We also gratefully acknowledge the financial supports from the European Integrated Center for the Development of New Metallic Alloys and Compounds (ECMetAC), the Université de Lorraine, the Métropole du Grand Nancy, Edwards Company and Vinci Technologies.

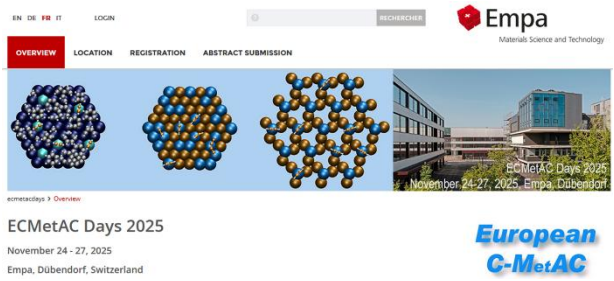
The next International Conference on Quasicrystals (ICQ17) will be held in Sendai, Japan, in 2028.

Vincent Fournée, Conference Chair.

Julian Ledieu, Conference Co-chair.

Upcoming Events

ECMetAC Days
24th -27th of November 2025



We invite you to attend the ECMetAC Days 2025, which will take place at EMPA, Dübendorf (Switzerland) from 24th to 27th November 2025. The conference is a continuation of the series ECMetAC Days, organized annually by a member institution of the European Integrated Center for the Development of Metallic Alloys & Compounds (ECMetAC, https://www.ecmetac.eu/). The ECMetAC Days 2025 are organized by Dr. Roland Widmer.

The ECMetAC Days 2025 will provide an excellent opportunity to present and get acquainted with the latest results in the field of newly discovered metallic alloys and compounds. The topics include formation, stability, synthesis, structural and chemical characterization, physical, chemical and mechanical properties, surfaces and thin films, catalysis, theory, applications and new frontiers in metallic materials. The materials of interest are (but are not limited to) conventional crystalline intermetallics, complex metallic alloys, quasicrystals and other aperiodic solids and soft matter, metallic glasses, high-entropy alloys, intermetallics for catalysis, correlated-electron systems, thermoelectrics, magnetocalorics and related materials. The topics are highly interdisciplinary and include mathematics, physics, chemistry, metallurgy and materials science.

ECMetAC Workshop

Innovative Researcher: Discovering the Expert in Yourself

Nov. 24th 2025, Dübendorf, Switzerland

„Innovative researcher: ...“ – a series of workshops allows to 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 focused on:

- Reclaiming the inner expert – recognizing our unique strengths. Here the goal is to help participants to identify their inner resources and key strengths that support their growth as researchers and leaders.
- Reframing self-doubt – transforming the inner critic. Here, our goal is to recognize and reframe common patterns of self-doubt, such as imposter syndrome or perfectionism, and to learn how to manage them consciously.
- Calm mind, clear message – regulating stress and strengthening presence. Here the goal is to introduce simple and effective techniques for reducing tension and improving focus, especially before presentations, important conversations, or evaluation sessions.

During our workshop, we will meet with Joanna Janowicz (emotional intelligence and resilience expert) to learn how to enhance the ability to represent oneself. The same, together we will train strengthening the mindset of the innovative researcher.

Related Upcoming Events

IUCr 2026, 11th-18th August 2026, Calgary, Canada

28th Congress and General Assembly of the International Union of Crystallography, 18th – 25th 2029, Berlin, Germany

Missing Content?

If you have any news items for circulation, either on our website https://ecmetac.eu/ or in this newsletter, please send them to Julian Ledieu (julian.ledieu@univ-lorraine.fr).

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