European CMetAC

ECMetAC Newsletter No. 14

January 2025

Dear colleagues of the ECMetAC network,

On behalf of the board of directors, we wish you a Happy New Year 2025! We hope that this year will be marked by great projects, fascinating results, new collaborations and above all, good health.

After celebrating in style the 15th anniversary of our consortium in Zagreb last November, it is now time to prepare ourselves for the next events. Following the great Euroschool 2024 that took place in Jülich, our young scientists will meet again in September in Dresden. This time, the Euroschool will be joint with the 6th International School on Aperiodic Crystals. Then and for the first time, the ECMetAC days 2025 will be organised at the Empa in Switzerland in November.

2025 will also be marked by the retirement of Prof. R. McGrath from his position of Secretary General after serving the consortium for 12 years. We would like to take this opportunity to thank him warmly for the great work accomplished. We are looking forward to working with his successor Dr. Hem Raj Sharma from the University of Liverpool.

During the year, online ECMetAC workshops will be organised and we invite you to visit regularly our website to keep up-to-date with the latest news.

Good start to all of you for this new year and we are looking forward to welcoming you in 2025 in Dübendorf and Dresden.

Best wishes,

Julian Ledieu, Ronan McGrath,
Marc Armbrüster, Jean-Pierre Celis
and Émilie Gaudry

The Euroschool 2024 in Jülich

The 2024 ECMetAC Euroschool was organized by Marc Heggen, Marc Armbrüster and Marie Göcking and took place at Forschungszentrum Jülich, Germany, from November 4 to 8, 2024. The theme of the 2024 Euroschool was Advanced Synthesis and Characterization. It was attended by 30 participants; lectures were given by Marc Armbrüster, Joachim Mayer, Michael Feuerbacher, Paul Paciok, Marc Heggen, Saleh Gorji, Robert Endert, Janez Dolinsek, Emilie Gaudry, Astrid Besmehn and Joachim Pasel.

Synthesis techniques of intermetallic compounds including bulk and single crystal growth as well as nanoparticle synthesis were covered. Advanced characterization techniques included among others various electron microscopy techniques (TEM, HR-TEM, STEM, SEM, EDX). A special focus was placed on modern in-situ analysis, the latest developments in electron energy loss spectroscopy (EELS) and four-dimensional scanning transmission electron microscopy (4DSTEM). Surface and interface analysis using Photoelectron spectroscopy (XPS) and Secondary Ion Mass Spectrometry (SIMS) were covered, as well. Lectures were complemented by step-by-step tutorials and hands-on lab exercises using modern aberration-corrected transmission electron microscopes at the Ernst Ruska-Centre. Lab

tours to the single crystal growth lab and the Helmholtz Nano Facility and a poster session were held. Anneliese Wirth & Gaurav Pransu received an award for the best poster presentation. Additional financial support from Ametek, Inc. and DENSSolutions B.V. is gratefully acknowledged.

Looking back at ECMetAC Days 2024 in Zagreb

The annual ECMetAC Days 2024 conference took place in Zagreb, Croatia, at the Institute of Physics from November 25 to November 28. This marked the second time the conference was held in Zagreb, following the C-MAC Days in 2014. This year's event was co-organized by Mario Novak from the Department of Physics, Faculty of Science (PMF), University of Zagreb, and Petar Popčević from the Institute of Physics.

The conference was officially opened with greetings from Osor S. Barišić, Director of the Institute of Physics, and Emil Tafra, a representative of the Department of Physics (PMF). Julian Ledieu, Director of ECMetAC, then formally launched the event. This year's gathering brought together 70 participants from across Europe, nearly half of whom were young scientists, including PhD students and postdoctoral researchers. It is encouraging to note that gender balance was significantly more evident among the young scientists.

The program included 34 oral presentations, divided into eight sessions, covering a range of topics such as: Development of new metallic compounds, Physical and chemical properties, Surface properties of metal alloys, Energy and quantum materials, Intermetallic catalysts, Complexity and high-entropy alloys. Additionally, 23 posters were presented during the poster session.

ECMetAC Days 2024 marked the 15th edition of the ECMetAC (formerly C-MAC) Days conference series. To commemorate this milestone, the first session after the opening was dedicated to the history and development of the Centre. Jean-Marie Dubois gave the opening lecture, tracing the origins of ECMetAC as the successor to the European Network of Excellence (NoE) "Complex Metallic Alloys." This was followed by talks from Yuri Grin, the Centre's first Deputy CEO, and Julian Ledieu, its current CEO.

A special session was dedicated to Ana Smontara, who significantly contributed to the study of charge and heat transport in complex systems. Her collaborations with numerous European (and international) laboratories began even before the establishment of the Centre. Ana's efforts were instrumental in securing membership for the Institute of Physics – and consequently, other Croatian institutions – in the Centre. Speakers in this session included Neven Barišić; Janez Dolinšek, a long-time collaborator of Ana within ECMetAC; Peter Gille, who delivered his final talk (again, for the second time); and Ante Bilušić, Ana's first PhD student.

The concluding remarks were delivered by Ronan McGrath, the long-serving Secretary General, who has now retired from his position. He summarized the two days filled with engaging lectures and fruitful discussions. During the conference dinner, four Young Scientist Awards were presented - details can be found below.

On the afternoon of November 25, an ED&I RAD workshop, organized by Magdalena Wencka, was conveniently held ahead of the conference opening.

Finally, it was announced that ECMetAC Days 2025 will be hosted by EMPA in Dübendorf, Switzerland.

RAD Equality, Diversity and Inclusion in Material Science Workshop

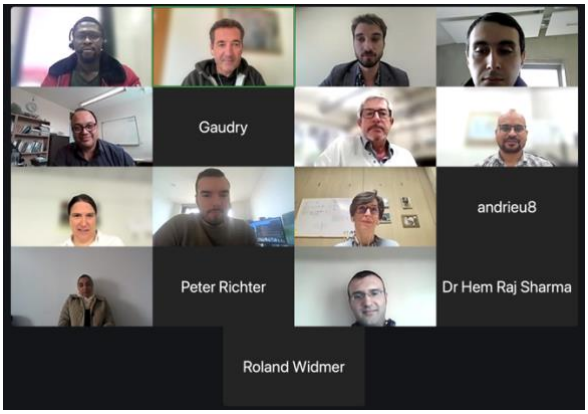
"Innovative researcher: how to make an impression when presenting research data"

„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 public speaking and skills of presenting scientific data. In the first part of our meeting, we met with Joanna Janowicz who is an expert on public speaking in business. She is the originator and the 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 (Poland) entitled „Extreme Public Speaking". Joanna taught us how to eliminate harmful stress and fear that appear standing in a front of the audience and how to communicate with our recipients. We had also an opportunity to get hints from scientists of different generations who shared their secrets and helped us to make an impression when presenting research data. Dr. Yuki Utsumi from Institute of Physics in Zagreb (Croatia) introduced us to the secrets of a properly prepared presentation and shared with us how she deals with preparing her own lectures and with facing stress. Ahowd Yousef Alfahad from The University of Liverpool (SSRC, UK) who is a laureate of The ECMetAC Young Scientists Oral Presentation Award (ECMetAC Days 2023, Kranjska Gora, Slovenia) emphasized how important passion for science is when presenting the results of scientific research. Then Prof. Janez Dolinšek, the Head of the JSI High-Entropy Alloys Group (Jožef Stefan Institute, Ljubljana, Slovenia) reminded after Albert Einstein that "If you cannot explain it simply, you do not understand it enough" adding that things should be explained at a simple way but not to simply so as not to lose the scientific truth. At the end, each of us became aware of our strongest skills, which will support us when presenting scientific results.

Dr. Magdalena Wencka

Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Online Workshop for the RAD ASCI



A one-day workshop was organised by Dr Hem Raj Sharma on 1st October 2024 focusing on the surface properties of intermetallic compounds. This event formed part of the annual activities of the Research and Activity Domain on Atomic Scale Surfaces, Functional Coatings, Thin Films, and Interfaces (ASCI) under ECMetAC. The workshop covered the surface properties of a wide range of intermetallic compounds, including quasicrystals, shape memory alloys, high-entropy alloys, and intermetallic catalysts.
This workshop was a great opportunity to invite Dr. Francesca Casoli from the Institute of Materials for electronics and Magnetism (IMEM), Parma in Italy to present her work entitled *Microstructure as a key to control the properties of magnetic shape memory films*. The second invited speaker was Prof. Stéphane Andrieu from the Institute Jean Lamour (IJL), Université de Lorraine, in Nancy France to introduce the audience to *Epitaxial ternary compounds grown by MBE for*

spintronics applications. Along with these external invited speakers, the event was attended by researchers from various European institutes within ECMetAC. During his closing remarks, Julian Ledieu stressed the importance of such workshops in fostering research collaboration. He encouraged young researchers to take advantage of the Young Researchers Exchange Scheme for short-term research visits to ECMetAC member institutes.

RAD Development of new metallic alloys and compounds

We would like to acknowledge the remarkable scientific contribution of Prof. Peter Gille as well as his investment from early days within the network of excellence on Complex Metallic Alloys and then within ECMetAC. Due to retirement, Peter has stepped down as speaker for the RAD Development of new metallic alloys and compounds, leaving the position open for candidacy. Thank you so much Peter and we wish you a long and happy retirement.

If you are interesting or would like to get more information about the open position, please contact us.

New RAD on High Entropy Alloys

In 2024 the procedure to establish a new Research and Activity Domain (RAD) within ECMetAC has taken place, finalizing with the GB and GA accepting the candidacy of Assist. Prof. Dr. Primož Koželj from the Jožef Stefan Institute in Ljubljana as RAD speaker. The new RAD called “High-entropy alloys” will tackle high-entropy alloys (HEAs), multicomponent metallic systems where five or more elements randomly mix on a simple lattice such as fcc and bcc, as well as all related systems (medium-entropy alloys, intermetallics with a high-entropy site, high-entropy oxides, etc.). Topics to be explored will include discovery of new alloys; design and optimization of alloys; physical properties of the alloys such as magnetism and superconductivity (also in connection with the alloys’ structure); mechanical properties; micro- and nanoscale characterization; HEA surfaces and surface properties; theoretical investigations into HEAs; and likely many more yet to come.

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Awards

ECMetAC Euroschool Poster Presentation Award: Anneliese Wirth

Department of Chemistry, Faculty of Natural Sciences, Technical University Chemnitz, Chemnitz, Germany

"*Membraneless Direct Methanol Fuel Cell – A Material Quest*"

Anneliese Wirth is a PhD student in her second year in the research group of Prof. Armbrüster for Materials for Innovative Energy Concepts. As such her work is focused on the development of new and selective catalyst materials for direct methanol fuel cells that do not require a membrane to separate the two half spaces of the cell. Finding these highly selective catalysts presents a proper challenge. As possible materials she focuses on the class of intermetallic compounds. This is a fascinating class of compounds as they show interesting electronic properties and structures which are different from the elements that make up the compound. Understanding and then tuning their properties can help to identify very selective electrocatalysts for methanol fuel cells.
In her free time she likes to go outside for hiking and seeing impressive natural landscapes in the process. Otherwise, she very much enjoys reading as a way to clear her mind. Additionally, she does a lot of knitting/crocheting. She finds that her skills for handiwork also help her out a lot in the lab for doing precise tasks.

ECMetAC Euroschool Poster Presentation Award: Gaurav Pransu

Institute of Physics, Zagreb, Croatia

"Synthesis and Characterization of Intercalated Transition Metal Dichalcogenides"

Gaurav Pransu, is a third-year Ph.D. student at the Institut za fiziku in Zagreb. Gaurav's research, under the guidance of Dr. Petar Popčević, primarily focuses on magnetically intercalated transition metal dichalcogenides. The goal is to understand the effects of intercalation on the host compound and the interactions between metallic and newly formed magnetic subsystems, which influence the ground state formation. His study examines various intercalated systems with different transition metals, exploring their crystallographic, magnetic, and electronic structures. One area of interest is the impact of disorder among intercalated atoms, investigated through a comparative study of Ni_xNbS_2 ($0<x<0.6$). The other point of interest is the effect of complex magnetic structures in $Co_{1/3}TaS_2$ and $Co_{1/3}NbS_2$ on their physical properties, especially transport properties.

At ECMetAC Euroschool, Gaurav presented

the synthesis process and results for Ni_xNbS_2 ($0<x<0.6$) and $Co_{1/3}TaS_2$. The samples were synthesized using the Chemical Vapor Transport method, and their transport and magnetic properties were reported up to 7T. It was found that the transition temperature for $Co_{1/3}TaS_2$ was 45K and for $Ni_{1/3}NbS_2$ was 95K. Gaurav also reported the band structure of $Ni_{1/3}NbS_2$ using ARPES measurements and DFT calculations. A comparative study of Ni_xNbS_2 ($0<x<0.6$) was conducted to understand the effect of intercalation ratio on the system's transport and susceptibility measurements.
Gaurav also contributed to the organization of ECMetAC 2024, which was hosted at his home institute. Outside of his academic work, he enjoys traveling and playing table tennis in his free time.

Award Ceremony - ECMetAC Days 2024

Our Laureates (from the left): Jože Luzar (Jožef Stefan Institute, Ljubljana, Slovenia), Jacob Wright (Empa, Dübendorf, Switzerland), Oksana Karychort (Ivan Franko National University of Lviv, Ukraine and visiting MPI CPfS Dresden), and Peter Richter (Chemnitz University of Technology, Institute of Physics & MAIN, Cheminitz, Germany).

ECMetAC Young Scientists Oral Presentation Award: Oksana Karychort

Ivan Franko National University of Lviv, Ukraine and visiting MPI CPfS Dresden

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

Oksana Karychort is a third-year PhD student at Ivan Franko National University of Lviv, Ukraine. She is currently a recipient of a DAAD scholarship, conducting research in the REALM group at the Max Planck Institute for Chemical Physics of Solids in Germany.

Oksana's research focuses on synthesizing novel ternary arsenides and phosphides, exploring their crystal structures, and studying their physical properties. Her work aims to advance the scientific community's understanding of these complex materials, which hold promise for applications in electronics and cutting-edge technologies. Through her research, Oksana aspires to develop new materials with tailored properties.

In her free time, Oksana enjoys reading and traveling. Reading is one of her greatest passions, and she has a particular interest in both scientific literature and fiction. She finds that reading broadens her horizons and nurtures her curiosity. Traveling is another activity she loves, whether it involves exploring vibrant cities or immersing herself in nature. Through her travels, Oksana experiences different cultures, meets new people, and draws inspiration for her academic and personal endeavors.

ECMetAC Young Scientists Oral Presentation Award: Jacob Wright

Empa, Dübendorf, Switzerland

"Asymmetric Heterogeneous Catalysis of Chiral Molecules on PdGa{111}"

Jacob Wright received his MSc. in Materials Science from ETH Zürich in 2023. In October of 2023, Jacob began his PhD with the nanotech@surfaces Laboratory at Empa in collaboration with EPFL. There, he pursues the development of chiral intermetallic compounds (i.e. PdGa) as a platform for selective asymmetric heterogeneous catalysis of chiral molecules. Toward this end, he utilizes scanning probe techniques such as STM and nc-AFM, spectroscopy methods including XPD, ARPES,

and also LEED-I(V). The project lies at the fascinating intersection of crystallography, nano-scale physics, and chemistry, which means there is no shortage of new things to learn. One aspect he finds enjoyable about the work is its technical and hands-on nature, requiring the maintenance of ultra-high vacuum systems. He is additionally working on a machine learning algorithm to help speed up the process of analyzing thousands of molecules from STM scans.

In his free time, Jacob likes to go for runs in the scenic hills around Zurich, and experiment in the kitchen by trying new dishes from around the world. More recently he has picked up astrophotography, which is a relaxing outlet.

ECMetAC Young Scientists Poster Presentation Award: Jože Luzar

Jožef Stefan Institute, Ljubljana, Slovenia

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

Dr. Jože Luzar is a prominent researcher specializing in the study of advanced metallic materials, with a focus on physical properties, magnetism, and nanostructure-driven properties of high-entropy alloys (HEAs). His extensive work spans cutting-edge topics like magnetic softness, vanishing magnetostriction, superconductivity, and structural properties of complex alloys. Dr. Luzar has contributed to numerous high-impact journals and international conferences, often exploring the functional integration of materials for innovative applications, such as supersilent devices and energy-efficient technologies. His interdisciplinary approach bridges fundamental research with practical applications, pushing the boundaries of material science.

In recognition of his work, Dr. Luzar received the award for "The Young Scientist Best Poster Presentation" at ECMetAC Days 2024 in Zagreb. His award-winning poster, titled *Physical Properties of Supersilent (GaNi)xCoCrFe High-Entropy Alloys*, highlighted innovative research on materials with unique magnetic and acoustic properties.

Beyond his research, Dr. Luzar is passionate about sports, particularly sport climbing and boulder climbing, where he finds both physical challenge and mental focus—a balance that mirrors his commitment to precision and perseverance in scientific work.

ECMetAC Young Scientists Poster Presentation Award: Peter Richter

Chemnitz University of Technology, Institute of Physics & MAIN, Cheminitz, Germany

"Growth and characterization of CoCrFeNi on $LaAlO_3$ substrates"

I earned both my bachelor's and master's degrees from TU Chemnitz in the Technical Physics group under the guidance of Prof. Thomas Seyller.

My experimental work was focused on the growth and characterization of graphene on SiC(0001) and the intercalation of the graphene-SiC interface using Pb, which facilitated the creation of new 2D materials.

To start my PhD work, I remained in the same group but transitioned to high entropy alloy (HEA) thin films to explore a new research area. The preliminary work of our group focused on the epitaxial growth of CoCrFeNi films on substrates like MgO(100) and Al_2O_3(0001) using DC magnetron sputtering. To improve film quality, I studied the growth of CoCrFeNi on $LaAlO_3$, which offers a better lattice match. This work involved investigating the atomic and electronic structure of the CoCrFeNi by means of bulk- and surface

sensitive techniques, the results of which were presented at the CMAC.

Our future projects will focus on exploring oxygen adsorption on HEA surfaces as well as their potential as electrocatalysts for processes such as the hydrogen evolution reaction.

Through my work in Prof. Seyller's group, I have not only gained valuable insights into the fields of graphene and HEAs but also experienced a great and productive work environment with my colleagues.

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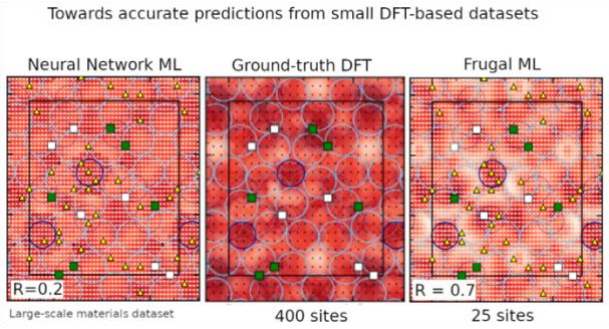
Partner Presentation: eXplor center @ Univ. Lorraine

eXplor is the high-performance computing facility of the University of Lorraine. Its main objective is to bring together the technical and human resources needed to support research in all areas involving intensive computing needs. It is open to people from the University, as well to those from associated scientific centers (CNRS, etc).

Explor Room @ Univ. Lorraine Datacenter

The center has recently relocated to a dedicated data center building, where it now benefits from an integrated environment. This new setup allows for enhanced collaboration, further boosting the center's computational capabilities. While eXplor may not rival the largest national supercomputing centers, it offers substantial capabilities, positioning itself as a valuable asset for research projects across various disciplines. Currently, nearly 400 users are involved in over ~90 active projects. Over 70 million compute hours have been used last year, contributing to a steady stream of impactful research output.



Adsorption Energy Maps generated from Density Functional theory, frugal Machine Leaning and Deep Learning.
Nathan Boulangeot, Florian Brix, Frédéric Sur, and Émilie Gaudry, *Journal of Chemical Theory and Computation* ***2024*** *20 (16), 7287-7299.*

The center is built around a shared resource model, maximizing computational power. A rich and diverse offer of codes and tools are available for simulation, analysis, and modeling. Excitingly, the University is also expanding its computational capacity with the upcoming arrival of machines as part of the GENI (Grand Est Numérique Intensif) and ENACT (European Center for Artificial Intelligence Through Innovation) projects, to cite a few. Thanks to its advanced resources and dedicated support, the center plays a key role in producing high-impact scientific results, advancing knowledge across a wide array of fields.

The University is looking for a **Support Engineer** to join our dynamic team responsible for operations and technical support. This role offers the opportunity to work in a stimulating environment where you can leverage your technical skills while actively contributing to the continuous improvement of internal processes.

Recruitment Process: The recruitment process will follow the rules and procedures set by the University. We encourage qualified candidates to directly contact our board: explor-directoire@univ-lorraine.fr

More Details: Full details about this position will be available soon on our website.

https://ecmetac.eu/

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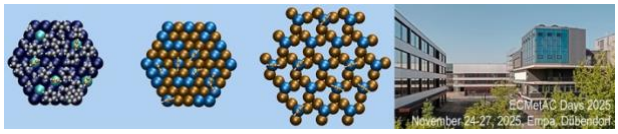
Upcoming Events

ECMetAC Euroschool 2025 in Dresden 1st till 5th September 2025

The next ECMetAC Euroschool will be joint with the 6th International School on aperiodic Crystals. The school will cover several topics ranging from an introduction to aperiodic crystals, superspace symmetry, refinement of modulated crystals to high entropy alloys and incommensurate magnetic systems to name a few. With an impressive list of world-class experts, the lectures will target mainly Ph.D. students, and doctorate fellows. It will be a great opportunity for young researchers to not only attend state-of-the-art lectures but also to extend and establish a network in the field. For more information, please visit the dedicated website. Contacts: Dr. E. Svanidze / Prof. Dr. T. Doert.

Next ECMetAC Days – November 2025

The 16th edition of the ECMetAC Days will be organized for the first time by the nanotech@surfaces Laboratory at Empa, Switzerland, from November 24 to 27, 2025.



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.

The interest of the participants in scientific equipment will cover a wide range from UHV surface analytical tools like Scanning Probe Microscopy, Photoemission Spectroscopy and related UHV preparation methods, to high resolution magnetic and electrical properties characterization. Optical microscopy and spectroscopy techniques will be equally represented as chemical synthesis and computational modelling.

Local organizing committee
Dr. Roland Widmer
Christine Tran

For more information, please visit the website.

Related Upcoming Events

ICQ16 – The 16th International conference on Quasicrystals

22th -27th June 2025, Nancy (France)

Abstract submission is now open!

We are pleased to invite you to the ICQ16 conference. This event will offer an excellent opportunity for researchers working on quasicrystals and related topics to discuss on emerging research, exchange ideas, establish a plural dialogue and encourage active collaborations with other research groups, hence promoting material science and engineering. This conference will bring together all the best scientists in the world to make a

major contribution about the recent developments in the field.

The conference will be held in Nancy, a magnificent ducal city located just 90 minutes from Paris and from Luxembourg. Nancy is the French capital of Art Nouveau, with an outstanding collection of 18th century monuments, including the beautiful royal square Stanislas inscribed on UNESCO's World Heritage List. It is also a lively student city, where you can enjoy a friendly atmosphere with many bars, café terraces, restaurants and museums. Please visit the website form more information and the area/topics covered.

EUROPACAT 2025 – Trondheim, Norway

The event from 31st August till 5th September 2025 will be the 16th European Congress on Catalysis under the auspices of the European Federation of Catalysis Societies (EFCATS) and organized as a joint effort of the Nordic Catalysis Societies. A special session dedicated to ***Intermetallic compounds in catalysis*** will be chaired by Prof. Marc Armbrüster and Dr. Iryna Antonyshyn.

ECM35 – Poznań, Poland

The 35th edition of the European Crystallographic Meeting initially planned to be held in Lviv, Ukraine has been relocated to Poznań. The conference will take place from 25th till 29th of August 2025 with the registrations opening by 3rd February 2025. For more information, please visit the website.

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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Imprint

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