European CMetAC

ECMetAC Newsletter No. 17

August 2026

Dear colleagues of the ECMetAC network,

Greetings from the Board of Directors!

This 17th edition of the ECMetAC Newsletter highlights the activities and achievements of the ECMetAC network over the past six months.

Looking ahead, following our successful meeting at EMPA in Dübendorf, Switzerland, the next **ECMetAC Days** will take place at AGH University of Kraków from **23–26 November 2026**. We are pleased to announce that preparations for the event are well underway. Notably, AGH University also hosted the C-MAC Days in 2012. We look forward to welcoming all of you to Kraków for another exciting scientific meeting and an excellent opportunity to strengthen collaborations across the network.

Meanwhile, we would like to thank Prof. Andreas G. Boudouvis from the National Technical University of Athens for his continued contribution to the ECMetAC network. We are also delighted to welcome his colleague, Prof. Costas A. Charitidis, as a new member of the network from the institute.

We wish you all an enjoyable summer despite the severe heatwaves and devastating wildfires that have affected parts of southern France and Spain. We also hope you have thoroughly enjoyed the excitement and spirit of the FIFA World Cup, whether cheering for your favourite team or simply sharing in the celebrations.

Enjoy reading this newsletter and look forward to meeting many of you in Kraków.

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

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ECMetAC Days in Kraków, Poland, 23-26 November 2026

The next **ECMetAC Days** will be held in Kraków at AGH University of Kraków from **23–26 November 2026**. Registration is now open.

The conference venue, along with catering and accommodations, will be conveniently located on the AGH campus, near the Old Town.

The conference provides an excellent opportunity to present the results of scientific, experimental, and/or theoretical research, promote young scientists, PhD students, and students in gaining experience in scientific presentations, and establish and strengthen collaboration between partner laboratories or departments operating in the areas of research and activities (RAD) and beyond.

The conference covers the formation, stability, synthesis, properties, applications, and emerging frontiers of metallic materials. Materials of interest include conventional and complex intermetallics, quasicrystals and other aperiodic

The conference venue (left) and the old town of Krakow.

materials, metallic glasses, high-entropy alloys, strongly correlated-electron systems, and energy and quantum materials, including thermoelectric and magnetocaloric materials. Research topics span structural and chemical characterization, surface and thin-film science, catalysis, and computational modeling. The conference brings together perspectives from physics, chemistry, metallurgy, mathematics, and materials science.

The ECMetAC Days 2026 is organized by Prof. Janusz Tobola and the team from the Department of Condensed Matter Physics (Faculty of Physics and Applied Computer Science, AGH University).

Don't miss the important deadlines.

Date	Event
May 1	Registration and abstract submission open
September 20	Registration and abstract submission deadline
October 18	Notification of presentation type (oral or poster)
November 10	Final programme available online
November 23	Conference begins

Further information about the event is available on the conference website: `https://ecmetac.eu/ecmetac-days?view=seeminicontent&id=68`

For enquiries, please contact the organisers at: `ecmetac2026@agh.edu.pl`

Research and Activity Domains (RAD) Activities

RAD High-Entropy Alloys: Publications

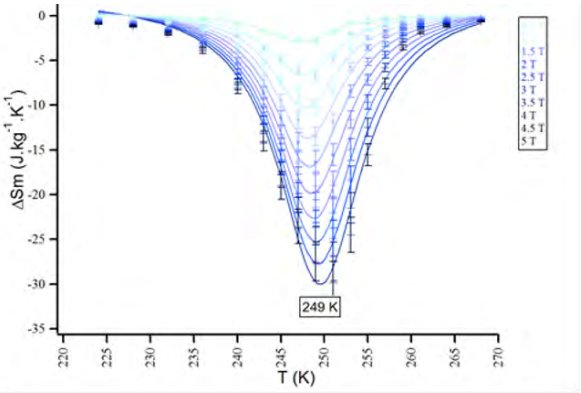
Chemical ordering and non-linear magnetic behavior: enhancing the magnetocaloric effect in FeMnNiGeSi high-entropy materials

ECMetAC members from the Institute Jean Lamour and AGH University, together with colleagues from Parma and Ljubljana, report detailed investigations of magnetocaloric high-entropy materials in the FeMnNiGeSi system, with and without manganese additions of up to 3 at.%. Their experimental studies, including powder X-ray diffraction (P-XRD), single-crystal X-ray diffraction (SC-XRD), and scanning transmission electron microscopy (STEM), combined with *ab initio* calculations within the KKR-CPA framework, demonstrate that FeMnNiGeSi-based materials do not exhibit a completely random atomic distribution over all lattice sites, as expected for ideal high-entropy alloys. Instead, they are more accurately described as high-entropy materials with chemical ordering between the transition-metal and metalloid sublattices. Incorporating this ordering into KKR-CPA calculations also provides a more accurate description of the magnetic moments and exchange interactions.

Small additions of 1–3 at.% Mn, combined with appropriate annealing, significantly enhance the already promising magnetocaloric performance. The isothermal magnetic entropy change increases by a factor of approximately 3.5, from $|\Delta S_m| = 9.2\ \mathrm{J\,kg^{-1}\,K^{-1}}$ in a magnetic field of 5 T to $35\ \mathrm{J\,kg^{-1}\,K^{-1}}$. An additional benefit of this chemical tuning is an increase in the Curie temperature to approximately 263 K, bringing it closer to room temperature and making these materials more attractive for magnetic refrigeration applications.

Furthermore, chemical tuning can transform the first-order magnetostructural transition into a second-order magnetic transition, thereby re-

ducing hysteresis and suppressing the associated volume change. These improvements address two of the major challenges limiting the practical implementation of magnetocaloric materials.



Calculated isothermal magnetic entropy change, ΔS_m, for 1 at.% Mn-doped FeMnNiGeSi around the second-order magnetic transition.

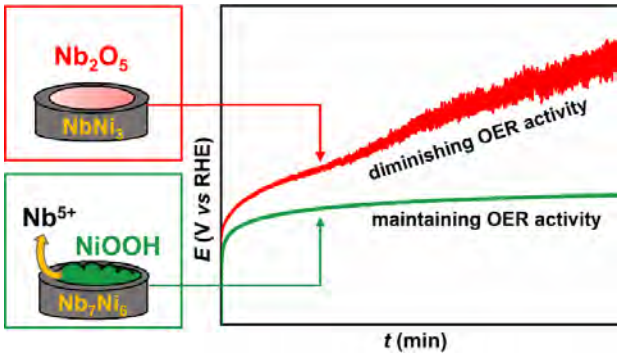
Reference: *Fournée et al., Materials Today Physics* ***65*** *(2026) 102128.*

RAD Materials for Catalysis: Publications

From Solid Solution to Intermetallic Compounds: Oxygen Evolution Reaction Activity Trends among Nb–Ni Phases

This study investigated the influence of crystal structure and chemical bonding on the electrocatalytic behavior of two Nb–Ni intermetallic compounds, Nb_7Ni_6 and $NbNi_3$, and compared their oxygen evolution reaction (OER) activity with that of the solid solution Nb_xNi_{1-x} ($x = 0.09$) and elemental Ni.

Under standard benchmarking conditions (chronopotentiometry at a current density of 10 mA cm^{-2} for 2 h), the Nb_xNi_{1-x} solid solution exhibited OER activity comparable to that of pure Ni. In contrast, the Nb_7Ni_6 intermetallic compound underwent rapid and progressive deactivation. Quantum-chemical calculations revealed that the local charge distribution in Nb_7Ni_6 makes the niobium atoms highly susceptible to oxidation, resulting in the formation of a dense Nb_2O_5 surface oxide layer. This passivating film inhibits charge transfer and significantly reduces catalytic performance.



Long-term oxygen evolution reaction (OER) performance of $NbNi_3$ compared with Nb_7Ni_6, the Nb_xNi_{1-x} solid solution, and elemental Ni. The dynamic surface evolution of $NbNi_3$ promotes the formation of catalytically active Ni (oxy)hydroxides while continuous Nb dissolution prevents surface passivation, resulting in superior catalytic activity and stability.

Unlike Nb_7Ni_6, the $NbNi_3$ intermetallic compound maintained its OER activity during the initial benchmark tests and exhibited excellent long-term stability under elevated current densities of 50, 100, and 200 mA cm^{-2} over a period of six days, outperforming elemental Ni. The dynamic surface state of $NbNi_3$ promotes the formation of catalytically active Ni (oxy)hydroxides while allowing the continuous dissolution of Nb from the surface, thereby sustaining high catalytic activity.

These findings demonstrate that the chemical bonding and electronic structure of Nb–Ni compounds directly govern their chemical behavior under OER conditions. Consequently, they determine the evolution of the catalyst surface and ultimately its electrocatalytic performance.

Reference: *Sevdaroğlu et al., Chemistry of Materials* ***38*** *(2026), 2788*

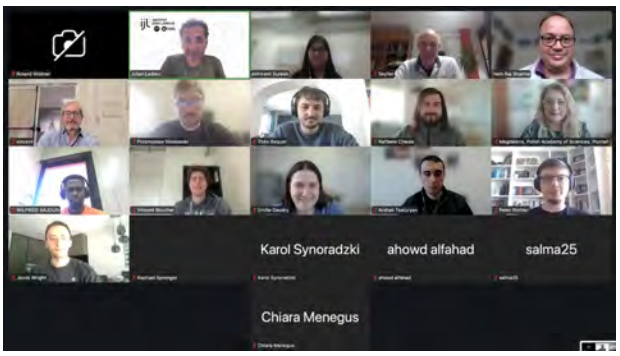
RAD Atomic scale surfaces and functional coatings, thin films and interfaces (ASCI)

Annual Workshop

A one-day online workshop was organised on 28 April 2026, focusing on the surface properties

of intermetallic compounds. The event formed part of the annual activities of the Research and Activity Domain (RAD) on Atomic Scale Surfaces, Functional Coatings, Thin Films, and Interfaces (ASCI) under the European Integrated Centre for the Development of Metallic Alloys and Compounds (ECMetAC).

The workshop covered the surface properties of a broad range of intermetallic compounds, including magnetic alloys, high-entropy alloys, energy materials, quasicrystals, and intermetallic catalysts. ASCI RAD members, including PhD and Master's students, presented their research alongside invited external speakers, Dr. Raffaele Cheula (Aarhus University, Denmark) and Dr. Elisabetta Arca (University of Liverpool, UK). Dr. Cheula delivered a presentation entitled *"Mechanistic and Kinetic Study of the Reverse Water–Gas Shift Reaction on Single-Atom Alloys,"* while Dr. Arca presented *"The Effect of Interfacial Instability on Battery Performance."* The workshop was attended by researchers from several ECMetAC member institutes across Europe.

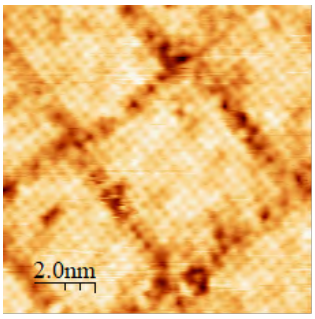


Participants of the ECMetAC ASCI RAD online workshop held on 28 April 2026.

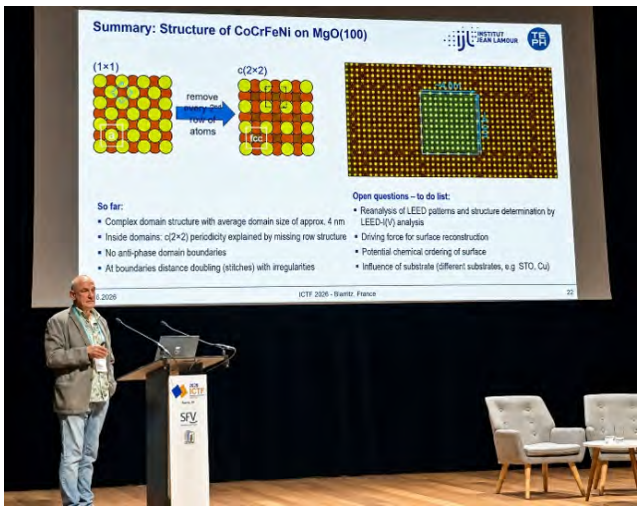
Dr. Julian Ledieu, CEO of ECMetAC, and Dr. Hem Raj Sharma, spokesperson for the ECMetAC ASCI RAD, highlighted the importance of such workshops in strengthening scientific collaboration within the ECMetAC network. Dr. Ledieu also encouraged early-career researchers to take advantage of the **Young Researchers Exchange Scheme**, which supports short-term research visits to ECMetAC member institutes.

Research Visits and Conferences

Prof. Thomas Seyller from TU Chemnitz spent one week at the Institut Jean Lamour, Nancy, France. Together with Julian Ledieu and Vincent Fournée, he investigated the surface structure of epitaxially grown CoCrFeNi(100) films using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). A surface structure was revealed that consists of a pattern of rectangular domains with lateral dimensions of a few nanometers. Within these domains, a c(2×2) missing-row reconstruction was observed. This successful collaboration demonstrates that multi-component metallic alloy surfaces can exhibit complex and intriguing structural behavior.



Scanning tunneling microscopy (STM) image of epitaxially grown CoCrFeNi(100) film.



Prof. Thomas Seyller giving a plenary talk at the 20th International Conference on Thin Films (ICTF2026).

He also gave a Plenary Talk at the *20th International Conference on Thin Films (ICTF2026)*, held in Biarritz, France, from 8–12 June 2026. In his presentation entitled *"Epitaxial High-Entropy Alloy Thin Films for Surface Investigations"*, he presented recent results from his

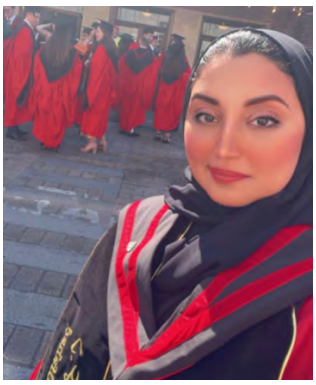
research group on the surface physics of CoCrFeNi high-entropy alloy thin films.

Dr. Hem Raj Sharma, from the University of Liverpool, also visited Institut Jean Lamour, Nancy, France during July 2026 under the Visiting Professor Scheme provided by Université de Lorraine. The visit focused on investigating the surface oxidation and atomic-scale surface structure of Ni-based intermetallic compounds using complementary surface-sensitive techniques, including XPS, LEED, STM, and UPS. This collaborative work advanced ongoing research into the surface properties of these materials and further strengthened the long-standing collaboration between the University of Liverpool and CNRS Nancy in the field of intermetallic surface science.

Dr. Hem Raj Sharma (right) with Dr. Julian Ledieu during his visit to Institut Jean Lamour.

Young Scientist Research Activities

Ahowd Alfahad from the University of Liverpool completed her PhD entitled *"Atomic Structure, Chemical Composition and Oxidation Behaviour of the Low-Index Surfaces of In_2Ni_3 Intermetallic Catalysts."* Her research was supervised by Dr. Hem Raj Sharma and Prof. Ronan McGrath and formed part of the collaborative research programme within ECMetAC. During her PhD, Ahowd actively participated in several ECMetAC Days and ASCI RAD workshops, and also undertook a research visit to a partner institute through the **ECMetAC Young Scientist Exchange Program**. These activities



Ahowd Alfahad on the occasion of her PhD graduation in Physics.

provided valuable opportunities for scientific exchange, international collaboration, and professional development, contributing to the successful completion of her doctoral research.

Salma Alnefaie, also from the University of Liverpool, visited Institut Jean Lamour, Nancy, France for a week in July under the ECMetAC Young Scientist Exchange Programme. During her stay, she studied oxidation bavahour of N-based intermetallic catalysts using STM, XPS, LEED and UPS.

The ECMetAC Young Scientist Exchange Programme provides financial support for early-career researchers to undertake short-term research visits to member institutes within the ECMetAC network.

Upcoming Events

- International Conference on High-Entropy Materials (ICHEM 2027), Paris, France, 27 June–1 July 2027, `https://ichem2027.com`.
- International Conference on Complex Orders in Condensed Matter (ICCOCM 2026), Evian, France, 27 September–02 October 2026 `https://iccocm.neel.cnrs.fr`
- 17th International Conference on Quasicrystals (ICQ17), Tohoku University in Sendai, Japan, June 2028, `https://icq17-sendai.org`
- 56th Journées des Actinides (JdA 2027), Tomar, Portugal, 6–9 April 2027 `https://journees-des-actinides.com/JdA2027`

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