

European CMetAC

ECMetAC Newsletter No. 9

July 2022

Dear colleagues of the ECMetAC network,

Summer greetings from the Executive Board!

Since the last newsletter the first events within our network took place in presence since the begin of the pandemic – slowly but steadily things are evolving toward normalisation!

Along this line one highlight in the network activity was the joint EuroSchool 2022 (together with the 5th International School on Aperiodic Crystals) which took place in Kutna Hora and was – especially concerning the very positive feedback by the participants – a huge success.

Looking ahead into the near future, the ECMetAC Days 2022 are planned as an on-site event in Split and will be accompanied by two workshops: One focusing on developments in the field of high entropy alloys dedicated to the 65th birthday of Janez Dolinšek and another one offering training for the PhD students within the network. Additional information can be found in this newsletter.

More details about these events and other news will be regularly posted on our website. Do not hesitate to send us your latest results or open positions or indeed any other important information for our members.

We are looking forward to seeing you soon!

Stay healthy and best wishes.

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

ECMetAC Days 2022 in Split



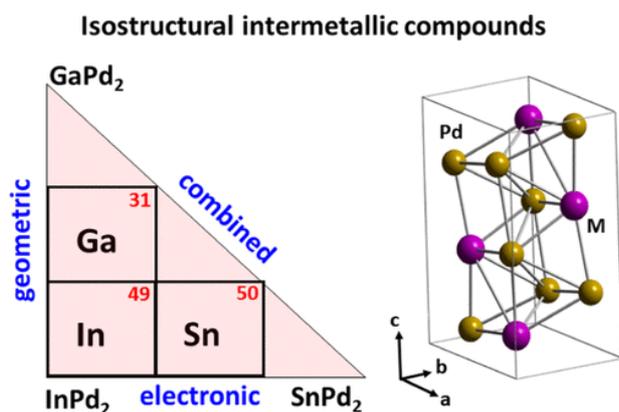
The ECMetAC Days 2022 will be organised from **21st till 24th November** by The University of Split, Faculty of Science. This year, we hope for the event to take place onsite. The main purpose of ECMetAC Days is to provide comprehensive information on recent results achieved within the current year of the ECMetAC network and to discuss directions for future research. More information regarding abstract submission and registration will be posted on our website very soon. The ECMetAC Days 2022 will be preceded and followed by satellite workshops.

News from the Research and Activity Domains (RADs)

RAD Materials for Catalysis – Use of Isostructural Compounds for Material Development Developed at MPI CPfS and Chemnitz University of Technology

Disentangling Electronic and Geometric Effects in Electrocatalysis through Substitution in Isostructural Intermetallic Compounds

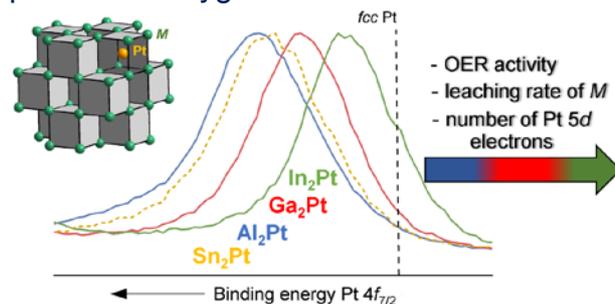
<https://ecmetac.eu/>



Efficient development of catalytic materials requires knowledge of the decisive parameters defining the catalytic properties. In multicomponent metallic catalysts, these are categorized as electronic and geometric effects, yet they are strongly interrelated. A systematic disentanglement can be achieved by fixing one parameter while altering the other, which becomes possible through the substitution in isostructural intermetallic compounds. This approach enables the evaluation of electronic or geometric contributions both individually and combined. Herein, this is achieved by substitution of indium (three valence electrons) with tin (four valence electrons) in the series $\text{In}_{1-x}\text{Sn}_x\text{Pd}_2$, which allows for a systematic variation of the total number of electrons per unit cell with only a minor variation of the unit cell parameters and thus the evaluation of the electronic effect. Geometric effects were evaluated by substitution of indium with gallium in the $\text{Ga}_{1-x}\text{In}_x\text{Pd}_2$ series, which allows for a systematic variation of the interatomic distances while maintaining the same number of valence electrons per unit cell and close atomic coordinates. By substituting gallium with tin in the $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$ series, both effects are combined and addressed simultaneously. The activity enhancement of the methanol oxidation reaction on the $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$ series is attributed to the synergy of the combined effects.

R. Zerdoumi, O. Matselko, L. Rößner, B. Sarkar, Yu. Grin, M. Armbrüster
J. Am. Chem. Soc. 144, **2022**, 8379.
<https://doi.org/10.1021/jacs.2c03348>

Isostructural $M_2\text{Pt}$ ($M = \text{Al}, \text{Ga}, \text{In}, \text{Sn}$) Compounds in Oxygen Evolution Reaction



Combining the stability of Pt under oxidative conditions with the ability of the main group element (M) to leach via the formation of the intermetallic compounds was applied as one of the possible ways to reduce the amount of noble metal and avoid the Ir-based materials for the development of the novel electrocatalysts for the oxygen evolution reaction (OER). Formation of the isostructural compounds allows to preserve the same crystal structure and track the influence of the nature of counterpart element onto the chemical bonding features, electronic state of Pt and, finally, on their OER performance and chemical behaviour under reaction conditions. The compounds $M_2\text{Pt}$ ($M = \text{Al}, \text{Ga}, \text{In}, \text{Sn}$) with the cubic anti- CaF_2 type of structure are characterized by strongly polar covalent interactions between M and Pt, accompanied by the noticeable charge transfer from M to Pt. The formation of intermetallic compounds leads to the modified electronic state of the Pt atoms, obvious from the shift of XP Pt 4f core levels and supported by the theoretical calculations. $M_2\text{Pt}$ compounds act as precursors for in situ formation of the dynamic surfaces, structure and morphology of which are strongly dependent on the nature of M and its leaching rate. Comprehensive experimental studies on $M_2\text{Pt}$ compounds were successfully combined with the computational studies, focused on the electronic structure and chemical bonding analysis.

A.M. Barrios Jiménez, A. Ormeci, U. Burkhardt, S.G. Altendorf, F. Kaiser, I. Veremchuk, G. Auffermann, Y. Grin, I. Antonyshyn
Sustainable Energy Fuels 5, **2021**, 5762.
<https://doi.org/10.1039/D1SE01190A>

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Reports

Focus Workshop TopCor22



The Focus workshop TopCor22, associated with the RAD "Energy and Quantum Materials", took place from April 11-13, 2022 and brought together 145 participants (50 on-site + 95 virtual) from 19 countries. Its main aim was to foster exchange between two largely distinct communities working on the weak and strong correlation regimes of topological quantum materials, to highlight emerging unifying themes of topology across the correlation spectrum and stimulate new ideas. For more information, see <https://www.pks.mpg.de/de/topcor22>

International School of Aperiodic Crystals & ECMetAC EuroSchool 2022

This year, the ECMetAC EuroSchool has been joined with the International School of Aperiodic Crystals. It has been organized on five days in Kutna Hora, a historical town located 80 km east of Prague. Experts in the field of aperiodic crystal have given lectures and organized tutorials on a step by step basis for each class of aperiodic crystals. This event has been an intense scientific and networking period and hopefully has helped researchers to gain a deep insight into different the field of aperiodic crystals. More than 60 persons have attended the school and the feedback is very positive.

Next year, the school will be organized in Sweden. More information will come later, but we hope that you will be able to participate to the fruitful event!



Upcoming Events

We list below some events that may be of interest to Network members:

2022 Joint European Magnetic Symposia, Hybrid conference – 24th-29th July 2022, Warsaw, Poland.

"JEMS covers a wide breadth of cutting-edge topics in magnetism and magnetic materials research, ranging from the fundamental to the applied."

Abstract submission deadline: 4th March 2022. <https://jems2022.pl/>

33rd European Crystallographic Meeting 23rd-27th August 2022, Versailles, France

Online registration opens on 15/02/2022

<https://www.ecm33.fr/>

IMCAT 2022 – 13th-15th September 2022 Chemnitz, Germany

"The symposium will cover all aspects of intermetallic compounds in catalysis in the fields of gas- and liquid-phase as well as in electro catalysis. This includes - but is not limited to - synthesis and characterisation, material development as well as catalytic properties."

<https://www.tu-chemnitz.de/chemie/mc/imcat/IMCAT.php>

<https://ecmetac.eu/>

Workshop@ECMetAC Days 2022 21st of November, Split, Croatia

It is our great pleasure to announce the 2nd dedicated ECMetAC workshop on „High-Entropy Alloys: from basic studies to industrial applications” that will be held in Split on 21st of November 2022. Similar to the 1st workshop topics cover formation and stability, surfaces and physical properties. The event takes place from 13:00 to 17.00 and is dedicated to the 65th anniversary of Prof. Janez Dolinšek, the Head of JSI High Entropy Alloys Group (Jožef Stefan Institute, Ljubljana, Slovenia). We cordially invite Jani’s friends and collaborators to share some cake.

Workshop@ECMetAC Days 2022 24th of November, Split, Croatia

On the last day of the ECMetAC Days 2022 in Split (24th of November) we propose especially to our young researchers (but not only) a workshop developing general innovative skills and dedicated to commercialization of scientific results “Innovative Researcher: How to design a marketable best-seller PhD thesis”. Thinking about particular “person” (end-user) to whom we would like to dedicate our scientific efforts we will use the Design Thinking (DT) process that consists stages of “empathize” (that means “to whom?”), “define” to know “why?”, “ideate” – to know “what?”, “prototype” (how?) and “test” (whether?). According to the DT method, to create an innovation we need to know our end-user and develop understanding of his/her situation, diagnose his/her needs, generate suitable ideas to solve particular problem, to make a suitable prototype and test it. The workshop will be guided by the DT Facilitator and Coach Katarzyna Gliszczyńska who is also an Innovation Consultant and a Senior Strategist and Dr. Magdalena Wencka (Innovation Manager and Design Thinking Moderator). Katarzyna Gliszczyńska is experienced in a development of new ideas and new

products (NPD). She dedicates her experience to business owners, managers and sellers, start-uppers, social innovators, artists and freelancers. Katarzyna was a consultant working for such concerns like IKEA and currently lives in Berlin.

We warmly invite you to join to our unique workshop, during which we will transfer the Design Thinking approach to a field of science to design a marketable best-seller PhD thesis or other scientific publication.

International Workshop on Exploration of Atomistic Disorder in Long-Range Ordered Systems and of Order in Disordered Materials

September 19th (Mon.) - 21st (Wed.), 2022
This meeting jointly organized by the National Japanese project 'Hyper-Ordered Structures Science' and the IRN Aperiodic will be held on an hybride form with on site workshop taking place in Grenoble.

More details on the web site <https://sites.google.com/hyperordered.org/disorder-order-ws/home>

Joint ICC-IMR, REIMEI and IRN Aperiodic international workshop on “Superconductivity, structural complexity, and topology of UTe₂ and aperiodic crystals”

The workshop will take place from November 30th to December 2nd 2022 in IMR, Tohoku University, Sendai, Japan.

This workshop is aimed at discussion and exchange of the recent progress on correlated electron materials and aperiodic systems between researchers and students. The focus is given to unconventional superconductivity in UTe₂ and other strongly correlated electron systems, as well as topological phenomena, structural complexity, disorder, CDW/SDW, crystal growth, and novel quantum phenomena.

Contact and abstract submission: Eteri Svanitze, eteri.svanidze@cpfs.mpg.de

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Missing Content?

If you have any news items for circulation, either on our website or in this newsletter, please send them to Julian Ledieu.

Newsletter Subscription

If you are interested in receiving the ECMetAC newsletter on a regular basis, please go to <https://ecmetac.eu/> and subscribe for the newsletter at the bottom of the webpage

Imprint

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CMAC-NSU V.Z.W.

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