

# European CMetAC

## ECMetAC Newsletter No. 2

August 2020

### Dear colleagues of ECMetAC,

The Covid pandemic has had deep impact on our daily life and of course our research. Many things that have been taken as granted have strongly changed – in science primary the way we communicate.

Many events were cancelled and many others took place virtually. Since our network is heavily based upon scientific and personal exchange, this change has deep impact. Fortunately, many things can be dealt with by telephone, e-mail or in virtual meetings. Nevertheless – and we think most of you will easily agree – communication in person is so much more than just exchange of information!

We still hope that the situation will improve until December so that the ECMetAC Days can take place as a normal conference – details on the event can be found on our webpage. A final decision will be taken in October with the primary consideration being the safety and wellbeing of our members. For many groups the pandemic resulted in a cut in funding. To enable the presence of many partners, the ECMetAC Covid fund has been established, providing travel grants for ECMetAC events.

As you might have seen, the new ECMetAC webpage has been launched. Other than the new layout, the content has been updated. The webpage offers two fields of participation: adding recent research highlights and posting job offers. In both cases, send a short e-mail with the content to Julian Ledieu ([julian.ledieu@univ-lorraine.fr](mailto:julian.ledieu@univ-lorraine.fr)).

Last but not least, this newsletter will be the last to be distributed manually – if you want to receive future newsletters from ECMetAC just subscribe at the bottom of the webpage <https://ecmetac.eu>.

Stay healthy and best wishes,

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

### ECMetAC Covid Fund

As we recognize that some organisations may have reduced resource due to Covid related financial constraints, the Board of Directors has agreed to make funding available to help cover travel expenses for partner organisations (up to a maximum of 500 € per partner organisation) to facilitate attendance at ECMetAC Days or a RAD workshop in 2020.

It is indeed important for our consortium to have at least one member of each partner present at the next ECMeAC Days in Split in December 2020.

The procedure is rather simple. Download the application form from the webpage (bottom, Travel & Reimbursement), fill and send to Jean-Pierre Celis ([Jean-Pierre.Celis@kuleuven.be](mailto:Jean-Pierre.Celis@kuleuven.be)) for approval by the Board of Directors. Important is to send the application form **in advance of any expense**.

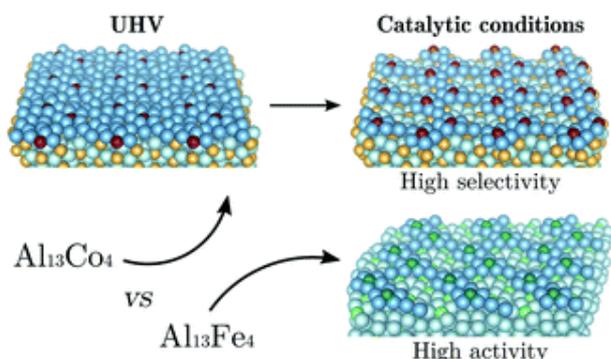


## News from the Research and Activity Domains (RADs)

### RAD Development of New Metallic Alloys and Compounds

#### Publication

Catalytic activation of a non-noble intermetallic surface through nanostructuring under hydrogenation conditions revealed by atomistic thermodynamics (DOI: 10.1039/D0TA01146K)

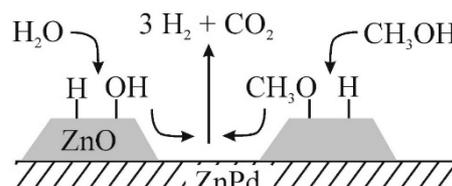


Transition metal ( $TM = \text{Fe}$  and  $\text{Co}$ ) aluminides of the  $\text{Al}_{13}TM_4$  stoichiometry have been previously demonstrated to exhibit high activities and selectivities in partial hydrogenation of alkynes and alkenes. Focusing on the  $\text{Al}_{13}\text{Co}_4(100)$  surface as a model catalyst for butadiene hydrogenation, the hydrogen-rich reaction conditions are predicted – based on DFT calculations and atomistic thermodynamics – to modify the relatively flat surface structure identified under ultra-high vacuum, in the form of highly cohesive clusters emerging from the bulk lattice. Unlike the flat one, this termination presents favourable adsorption properties, able to make it catalytically active and fully selective to butenes. In addition, its contrasted catalytic behaviour as compared to that of the reference  $\text{Al}_{13}\text{Fe}_4(010)$  surface – which is more active but less selective – is rationalized in terms of butadiene, butene and hydrogen co-adsorption properties. This work demonstrates that a realistic description of surface structures under reaction conditions is mandatory for designing new-generation catalysts based on the complex topology of intermetallic surfaces.

#### New Project

Elucidating dynamical atomic scale structural changes of ZnPd/ZnO methanol steam reforming catalysts

Cooperative project: Marc Heggen (Forschungszentrum Jülich) and Marc Armbrüster (TU Chemnitz)



Methanol steam reforming is an important reaction to provide hydrogen for fuel cell applications in a future methanol-based energy economy. The suppression of CO formation is one of the biggest challenges. In this regard, ZnPd/ZnO catalysts are very promising because they combine high selectivity (low CO formation) and high stability. The properties of this catalyst system and in particular its high selectivity depend crucially on the microstructure and elemental distribution. In particular, the distribution of Pd-rich and Pd-poor regions in the intermetallic ZnPd phase is critical for the formation of ZnO-rich regions and thus to the high selectivity of the material. Due to the high structural dynamics during methanol steam reforming, reliable structure-property relationships can only be established by combining *operando* investigations with atomic resolution and catalytic tests, both in a broad parameter field. The objectives of this project are to determine the catalytic properties of ZnPd / ZnO in terms of reaction and material parameters, to record the dynamic microstructure change under *operando* conditions in the electron microscope and to derive reliable structure-property relationships by linking the results from the catalytic and structural/morphological investigations.

PhD positions available  
Check [ecmetac.eu!](https://ecmetac.eu/)

# European CMetAC

## Reports

### ECMetAC EuroSchool 2020

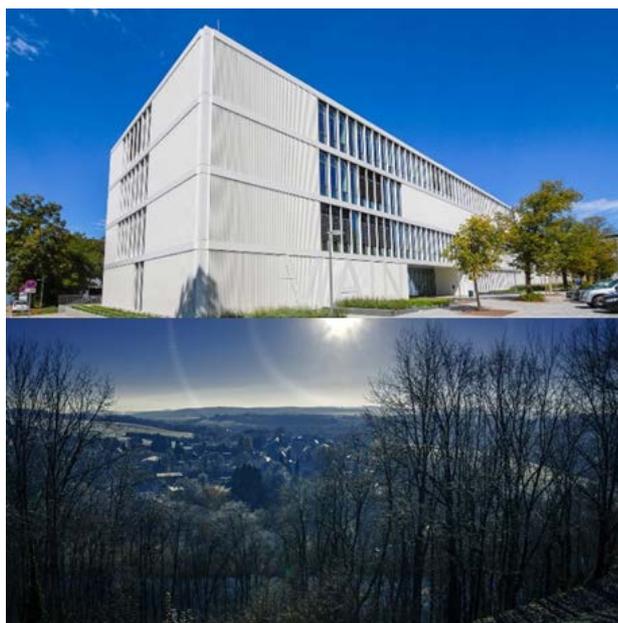
*Intermetallic Compounds – Advanced Synthesis and Characterisation (May 10<sup>th</sup>-16<sup>th</sup>, TU Chemnitz)*

This year's EuroSchool should have dealt with the synthesis and characterisation of intermetallic compounds – very unfortunately, the Covid situation forced us to cancel the event heavy-heartedly.

Intermetallic compounds have shown huge potential in different fields in the recent years, e.g. heterogeneous catalysis. For the EuroSchool a number of experts in the field of synthesis and characterisation of intermetallic compounds were ready to share their knowledge with the young researchers within the network and beyond, even reaching out to industry.

The last years have shown, that the ECMetAC EuroSchool is an important scientific and networking activity and serves as platform for young researchers to gain a deep insight into different fields.

This year's situation was very unfortunate and unprecedented, but the next EuroSchool will hopefully take place 2021 under normal circumstances!



### Young Scientist Exchange



In this new category, young researchers will report upon their experiences during a Young Scientist Exchange (YSE).

The tool offers to apply for a grant, which allows sending young researchers to other labs in the network. By this, additional expertise or methods not available at the home institution can be included in research. The aim of the tool is to directly enhance scientific exchange, enlarge the method knowledge of the young researcher and results quite frequently in common project proposals.

For each YSE a maximum of 1000 € can be granted and applying is straightforward and simple! Just fill in the "Application Form YSE" (<https://www.ecmetac.eu/travel-reimbursement>) and send it with the supporting documents to the treasurer of ECMetAC, Jean-Pierre Celis ([Jean-Pierre.Celis@kuleuven.be](mailto:Jean-Pierre.Celis@kuleuven.be)) for approval by the Board of Directors. Since the tool possesses copious funding, chances for success are high!

# European CMetAC

## Upcoming Events

### ECMetAC Days

Split, 7<sup>th</sup>-10<sup>th</sup> of December 2020



The next ECMetAC Days will be organised from 7<sup>th</sup> till 10<sup>th</sup> of December in Split. At this stage, the event is planned to take place on site and this situation will be reassessed in October. 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. Contributions will cover the field of metallic alloys and compounds ranging from basic to application-oriented research: Development of new metallic alloys and compounds, structure determination, stability as well as physical, chemical and mechanical properties. The field of topics is complemented by surfaces of complex metallic alloys, materials for thermo-electricity and magneto-caloric application, materials for catalysis, coating technologies as well as complexity in periodic and aperiodic metallic alloys and compounds (theory and experiment) and high-entropy alloys.

### EuroSchool 2021

The next EuroSchool will be organised in Liverpool, most probably in the period July-September 2021. At this stage, the event is planned to be held on site and this situation can be reassessed depending on the conditions. Details, including the programme, will be announced on the webpage <https://www.ecmetac.eu/>.

Started in 2006 within the CMA network of excellence, the aim of the EuroSchool is to provide a lecture-style background to young scientists, PhD students and graduate students in fields related to the activity domains of the ECMetAC network. Each one-week EuroSchool is dedicated to a specific topic matching with the

activity domains of the ECMetAC network. It includes lectures given on a step-by-step basis, as well as tutorials so as to practice what has been taught.

### Related Upcoming Events

#### *SCTE 2021*

*11<sup>th</sup>-16<sup>th</sup> of April 2021, Wrocław*

<http://scte2020.intibs.pl/>

#### *Kick-off meeting IRN Aperiodic*

*9<sup>th</sup>-13<sup>th</sup> of May 2021, Carry le Rouet*

<http://irn-aperiodic.grenoble.cnrs.fr/>

#### *Aperiodic conference*

*20<sup>th</sup>-26<sup>th</sup> of June 2021, Sapporo*

<https://wcp2-ap.eng.hokudai.ac.jp/aperiodic2021/>

### 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](mailto:julian.ledieu@univ-lorraine.fr)).

### 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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