

European CMetAC

ECMetAC Newsletter No. 11

July 2023

Dear colleagues of the ECMetAC network,

our splendid meeting in Split, Croatia, in November 2022 has nurtured further cooperation within the network. Leading to a number of short-term scientific missions, these activities have proven very fruitful in the past – and yes, funds are still available this year!

During the last meeting of the Board of Directors, the baton has been handed over from the founding directors Yuri Grin and Marc de Boissieu, who assisted the current Board of Directors with words and deeds to allow a smooth and sound transition.

The next face-to-face annual ECMetAC Days will take place from to in Kranjska Gora, Slovenia. Preparations are running full steam and Janez Dolinšek has already set up the webpage and registration is open. We are looking forward to Welcoming all of you at our yearly meeting in Slovenia!

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

Handover in the Board of Directors

Having built and smoothly sailed the ECMetAC ship ever since, Juri Grin and Marc de Boissieu left the Board of Directors as advisory members during the last Meeting of the Board in March 2023 in Paris.

While the waters were not always smooth, the ECMetAC network has shown its high resilience against detrimental influences and circumstances. A huge “Thank you!” to Marc and Juri for all the years they brought the network forward and strengthened the cooperation between the partners all over Europe.

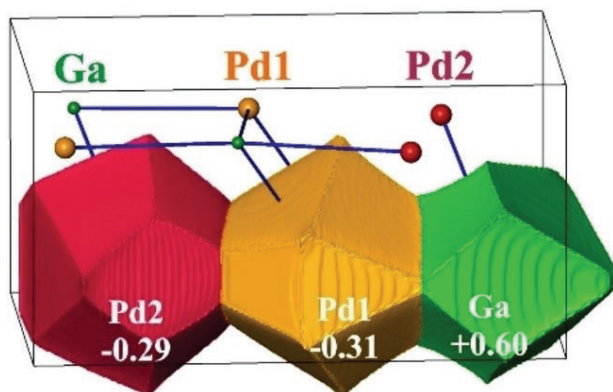


An impression of the Board of Director's Meeting in Paris in March 2023.

News from the Research and Activity Domains (RADs)

RAD Materials for Catalysis

Chemical Bonding in the Catalytic Platform Material $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$



The underlying reasons for the catalytic activity of $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$ ($0 \leq x \leq 1$) in the semi-hydrogenation of acetylene are analysed considering electronic structure and chemical bonding. Analysis of the chemical bonding shows pronounced charge transfer from the p elements to palladium and an unusual appearance of the Pd core basins at the surface of the QTAIM (quantum theory of atoms in molecules) atoms. The charge transfer supports the formation of the negatively charged palladium catalytic centres. Gallium-only-coordinated palladium atoms reveal a smaller effective charge in comparison with palladium species having tin in their coordination sphere. Within the empirical tight-binding approach, different influence of the E_{Pd} distances on the calculation matrix for the energy eigenvalues and the electronic density of states (DOS) leads to an S-like shape of the plot of the energy position of the $4d$ band centre of gravity versus substitution level x . The latter correlates strongly with the catalytic activity and with the varying charge transfer to palladium. The optimal value of negative palladium charge and the closest position of Pd d -states gravity centre towards the Fermi level correlates well with the catalytically most active composition x . Combination of all features of the chemical bonding and electronic structure allows more insight into the intrinsic reasons for the catalytic activity variation in the platform material $\text{Ga}_{1-x}\text{Sn}_x\text{Pd}_2$ ($0 \leq x \leq 1$).

A. Ormeci, E. Gaudry, M. Armbrüster, Yu. Grin, *Chem. Open* 11, **2022**, e202200185.

RAD Equality and Diversity in Material Science

ECMetAC Inclusion Policy: Good Practices

The ECMetAC network is entirely inclusive and takes care about well-being of its members. Thus, we have established the good practices to encourage meeting organizers to offer facilities dedicated to our researchers who have special needs (special room for feeding babies, rest rooms for pregnant women and health or medical purposes), their families and researchers with disabilities. Among others, the policy includes bringing support to participants of our network annual events who have dietary requirements. To get support, the participants should mention their special needs by filling the conference/school registration form. As good practice the above-mentioned issues (and others see our website: <https://www.ecmetac.eu/research?view=seerad&id=9>) will be implemented into event organization when possible (M. Wencka).

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Reports

Young Scientist Exchange



Ahowd Alfahad – I am in the second year of PhD studies at the University of Liverpool. Through support from the Network Young Scientist Exchange scheme, I had the opportunity to visit the Institute Jean Lamour for three weeks

in May 2023. The main topic of my studies is the surface structure of In_3Ni_2 intermetallic compounds. I used the X-Ray Photoelectron Spectroscopy (XPS) technique to study chemical structure of clean intermetallic compound of In_3Ni_2 under the supervision of Dr. Julian Ledieu, and Dr. Vincent Fournée. In my spare time I enjoyed looking around Nancy city.

ICQ15

The fifteenth [International Conference on Quasicrystals](#) was held in Tel Aviv from 19th-23th June this year, with ECMetAC as a supporter. The conference was a great success with participation and presentations from a number of ECMetAC institutions. A number of our delegates received young scientists awards from the International Union of Crystallography to support their attendance. Pictured are Liam Chandler and Naima Saadi from the University of Liverpool.



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Upcoming Events

ECMetAC Days

27th -30th of November 2023



We invite you to attend the ECMetAC Days 2023 conference, which will take place in Hotel Kompas in Kranjska Gora, Slovenia, from 27th to 30th November 2023. 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 (EC-MetAC, <https://www.ecmetac.eu/>). The EC-MetAC Days 2023 conference is organized by the Jožef Stefan Institute (JSI), Ljubljana, and the University of Ljubljana, Faculty of Mathematics and Physics. JSI is the organizer of a conference from this series for the second time, after C-MAC Days 2013 (the name of the conference has been changed to ECMetAC Days in the meantime).

ECMetAC Days 2023 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.

We cordially invite you to join us at the EC-MetAC Days 2023 in the beautiful Alpine resort of Kranjska Gora! (Janez Dolinšek)

ECMetAC EuroSchool 2023

Unfortunately recent events beyond our control have led to the cancellation of the intended EC-MetAC Euroschool in Wroclaw. We will work hard to ensure that next year's Euroschool will be organised very early to enable delegates to plan their attendance.

RAD Workshops

The ASCI Research and Activity Domain (RAD) will be organizing on 21st September with a full day meeting entitled Thin films and surfaces of high entropy alloys and intermetallic compound. The main objective of the workshop will be to share recent research progress within the ASCI RAD and explore possibility of collaboration or strengthen ongoing collaborations. The program will be available soon on our website and those interested to attend the workshop should contact the RAD speaker, Dr. Hem Raj Sharma (hemraj@liverpool.ac.uk).

Related Upcoming Events

26th Congress and General assembly of the IUCr, 22nd-29th August 2023, Melbourne, Australia.

Many micro-symposia will be dedicated to quasicrystal, aperiodic crystals, approximant, complex structure, disorder, and magnetic structures.

More information can be found [here](#)



ECM34

26-31 August 2023, Padova (Italy)

<https://www.ecm34.org/>

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CMD30, FisMat2023: 4th-8th September 2023, Milan Italy.



The 30th general conference of the Condensed Matter Division of the EPS will be held in Milan (Italy) on September 4-8, 2023, jointly organized with FisMat, the biennial conference of the Italian community of condensed matter physics, optics, liquids and soft matter.

Please visit the [website](#).

International conference on complex orders in condensed matter: aperiodic order, local order, electronic order, hidden order

24-29 September 2023, Evian (France)

<https://complex-orders.grenoble.cnrs.fr/>

SCTE 2024

16-21 June 2024, Prague (Czech republic)

<https://www.scte2024.org>

Missing Content?

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Newsletter Subscription

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