

## Solar2Chem News

## Dear Solar2Chem Friends,

The **Solar2Chem Conference** at ICIQ in Tarragona was a big success. The event spanned five days (18-22 September 2023), encompassing a variety of exciting activities: scientific talks, group discussions, workshops, awards, poster sessions, but also a piano concert from one of the ESRs and the celebrations of Santa Tecla Festival in Tarragona. In the last six months, **three scientific articles** were published by the Solar2Chem ESRs. Three of them also successfully concluded their project **defending their PhD thesis**. The next six months will be to the last ones of the project in which concluding the huge amount of work done by the entire consortium.

Read more details about these activities in the following sections!

Learn more about our project

**Solar2Chem Conference at ICIQ (Tarragona)** 



The scientific talks were given by pioneering experts of the field in photocatalysis and photo-electrocatalysis. A warm welcome remark was given by **Prof. Núria López**, our ICIQ partner Professor, **Prof. Emilio Palomares**, ICIQ Director, and **Prof. Pau Farràs**, the coordinator of the Solar2Chem project. **Prof. Harry Atwater** of California Institute of Technology and Liquid Sunlight Alliance (LISA), a partner of Solar2Chem, opened the floor for scientific discussions with his talk "*Coupled Microenvironment Artificial Photosynthetic Systems for Liquid Solar Fuels*". He discussed the strategies that LISA has been exploring to further photo-electrochemical conversion research. This was followed by a short presentation by **Sebastiano Gadolini**, our ESR from Johnson Matthey, who formally introduced the Solar2Chem Project and Consortium to the audience.

The second day started with an invited speaker from the industry, **Dr. Jacob Hjerrild Zeuthen** from Maersk, Denmark. He gave an overview of "Fuel Development for the Future Maritime Fleet" and discussed how solar-to-fuels technology can enter the industrial landscape in the perspective of alternative fuels for maritime transportation. After lunch, a representative of the Royal Society of Chemistry discussed how the RSC is "Transforming the Energy Publishing Landscape — RSC's Mission to

Advance Excellence in the Chemical Sciences". In the late afternoon, a keynote presentation was given by **Prof. Kazunari Domen** of University of Tokyo, Japan, and Shinshu University on "Photocatalytic Water Splitting and Green Hydrogen and Fuels Production Systems". As one of the pioneers in the field of photocatalysis, he also showed a functional PEC plant in Japan where they produce green hydrogen in large scale, discussing the constraints and the challenges involved.



Prof. Beatriz Roldán Cuenya of Fritz Haber Institute of the Max Planck kicked off the third day with her keynote presentation on "Beyond Static Models: Dynamics in Interfacial Catalysis". With her expertise in advanced characterization techniques for catalysis, she imparted key insights about the real dynamic state of these catalysts during operation. At the latter part of the day, Prof. Timothy Noël from the University of Amsterdam gave a different perspective in his keynote presentation entitled "From Batch to Flow: Advancing Synthetic Organic Chemistry through Technological Innovation". He proposed how to exploit light, flow chemistry, and machine learning in transforming the landscape for organic chemistry in the synthesis of specialty chemicals, not just fuels. The day concluded with a delightful surprise as Pavle Nikačević, an ESR from ICIQ, showcased his musical prowess in a captivating piano concert entitled "The PhD Sonata", demonstrating that the conference on sustainable fuels was not only an intellectual exchange but also a celebration of diverse talents, harmonizing science and art.

The fourth day began with a keynote presentation from **Prof. José Ramón Galán-Mascarós** of ICIQ with his talk on "Oxidation Catalysis and Renewable Fuels: Challenges and Beyond". He reminded the community about the challenging oxidation half-reaction and how his group is trying to solve it. With his talk, the

scientific part of the keynote presentations ended, and the schedule proceeded with presentations on Policy. **Dr. Philippe Schild**, Senior expert from the European Commission, discussed "Research and Innovation on Solar Fuels and Chemicals: Mission Innovation and the European Viewpoint", while **Dr. Luigi Crema**, the Hydrogen Europe Research President, presented his talk on "Hydrogen Europe Research and the Priorities for the Direct Solar Hydrogen Production".



During the last two days, the focus shifted towards the policy aspect of solar-to-chemicals where a workshop and roundtable panel discussion were held and were moderated by one of the ESRs, **Júlia T. M. Machado** from University of Galway. The workshop focused on "Future of Solar Chemicals and Fuels". The panelists were **Joan G. Fabra** (ICIQ alumnus from EU Commission, Political Landscape), Prof. **J.R. Galán-Mascarós** (Technology Development), and **Dr. Jacob Zeuthen** (Industrial landscape). Then, the roundtable "Solar Chemicals and Fuels Cluster" with the previous speakers **Luigi Crema** and **Philippe Schild**, with **Ann Magnuson** of the Swedish Consortium for Artificial Photosynthesis, **Frédéric Chandezon** from SUNERGY, and **Maria Rosa Palacin** from the International Battery Association. Aside from these, all 15 Solar2Chem ESRs presented their work orally.

Throughout the week, various presentations were given by attendees through oral or poster presentations. The event concluded with closing remarks from **Prof. Núria López** and **Prof. Pau Farràs**, after the awarding ceremony of the poster awards and scholarships. The best posters were given to three outstanding PhD students: **Enric Ibáñez Alé** of ICIQ, **Eva Jie Yun Ng Leon** of Institute of Advanced Materials - UJI Castelló (INAM UJI), and **Hanka Besic** of University of Galway. The RSC also granted scholarships to two deserving students: **Jing Yang** from University of Liverpool and **Samiksha Mukesh Jain** from INAM UJI. Lastly, the ESRs and the

attendees enjoyed the conference simultaneously with festivities during the week of Santa Tecla celebration in Tarragona, Spain.

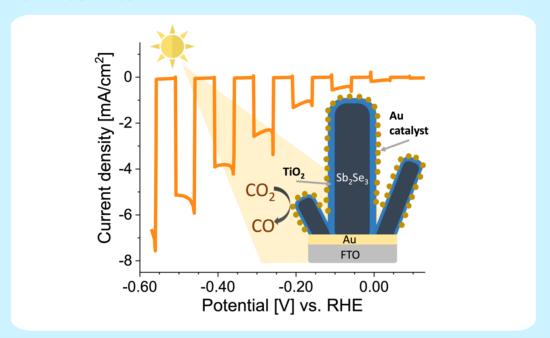


## Scientific publications in peer-reviewed journals

Francesca Lorenzutti and Prof. Sophia Haussener from EPFL published the paper "Morphology and Transport Characterization of Catalyst Layers for CO2 Reduction" on the *Journal of The Electrochemical Society*. Catalyst layers for electrochemical CO2 reduction were digitalized by FIB-SEM nano-tomography. They were analyzed to obtain a set of morphological descriptors and were considered as geometrical domains in direct pore-scale simulations to calculate tensors of effective diffusion coefficient, permeability, tortuosity, and effective ionic and electronic conductivity. The results provide a quantitative morphological analysis and a reliable set of effective properties to make device-scale homogenized modeling of GDEs more accurate and reliable.

Jokotadeola A. Odutola and Horatiu Szalad in a collaboration between Tampere University and UPV published the work "Long-Lived Photo-Response of Multi-Layer N-Doped Graphene-Based Films" on the Journal of Physical Chemistry C. N-doped graphene based films on quartz were prepared from chitosan pyrolysis in an inert atmosphere at different pyrolysis temperatures (900-1200 °C) and nitrogen doping levels. A comparative study of the opto-electronic properties of the films as a function of the doping level using ultrafast pump-probe spectroscopy and Drude-Lorentz modelling of the resulting spectra was realized. From the analysis, it was shown that the N-doped samples had an unprecedented long lived signal in the nanosecond range which could be attributed to trapping of photogenerated carriers.

John Mark Dela Cruz, Dr. Gergely F. Samu, Prof. Csaba Janaky and other researchers from Szeged University published the paper "Au-decorated Sb2Se3 photocathodes for solar-driven CO2 reduction" on EES Catalysis. This paper points toward the use of Sb2Se3-based photoelectrodes, a promising material in PEC water splitting, in solar CO2 reduction reaction applications. Au nanoparticle catalysts were deposited throughout the assembly having control over the size and morphology. Results show that the photocathode produced a photocurrent density of  $\sim$ 7.5 mA cm-2 at  $\sim$ 0.57 V vs. RHE for syngas generation, with an average faradaic efficiency of 25  $\pm$  6% for CO and 63  $\pm$  12% for H2.



## PhD thesis defenses

Solar2Chem project had three PhD thesis defenses:

- **Kathrin Naumann** (DTU) defended her thesis "Paving the way toward Photo-Electrochemical Carbon Monoxide Reduction";
- Alexey Galushchinskiy (MPICI) defended his thesis "Carbon Nitride: A Flexible Platform for Net Oxidative and Net-Neutral Photocatalysis";
- Pavle Nikačević (ICIQ) defended his thesis "Atomistic Insights into Photocatalytic Mechanisms: Modeling Selected Processes with Density Functional Theory".

Congratulations and all the best for a shiny future!













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