

MULTI-site organic-inorganic HYbrid CATalysts for MULTI-step chemical processes

Enjoy Reading our first Biannual MULTI2HYCAT Newsletter in 2021

Hello everyone. After a turbulent year, here comes another newsletter with an update of the activities of the last months.

Despite of difficult working period working period with drastic restrictions in all participating countries caused by COVID-19, we were able to achieve significant progress. Close collaboration among all partners was achieved through the use of virtual tools. Online meetings were a useful opportunity for extensive dialogue and an exchange of information. In all WPs fundamental results were obtained in the last months enabling to move forward to the last phase of the project. The MULTI2HYCAT project ends in June 2021.

Important notice: The planned industrial workshop had to be cancelled for good. Unfortunately, the current situation does not allow a reliable planning.

Summary and Highlights

• 9th biannual project meeting held in December 2020.

The 9th biannual MULTI2HYCAT project meeting was held virtually after 48 project months and the latest achievements were discussed.

Dissemination activities

In the last 6 months *three new scientific publications* have been issued. The *website* has been continuously updated.

EC reporting

5 deliverables were uploaded to the EU Participants Portal.

• Stakeholder Online Survey is still online.

This survey aims at collecting the opinions of specialists from the fields of catalysis, pharmaceutical chemistry and process engineering towards the MULTI2HYCAT approach and the future of chemical industry.

Your opinion is important to us! Please take part in this survey – your answers will allow us to better meet your expectations.

9th Biannual Project Meeting (virtual)

On 18 December the MULTI2HYCAT Consortium met virtually to expose the progress made during the previous 6 months. Regrettably, for the second time in a row the consortium cannot meet physically to discuss the next steps. Nevertheless, we tried to make the best of this situation. Despite the adverse circumstances, we worked effectively, but also enjoyed it.

Here is a brief summary on the research progress:

Since the last meeting, *five deliverables* were uploaded to the EC participant portal.

WP2 – Preparation of organic-inorganic precursors

BAM-BINAP precursors for hybrid materials have been prepared.



WP3 – Synthesis of multi-functional catalysts with hierarchical porosity

The synthesis of functional hybrid catalysts containing acid, basic, redox and/or chiral active sites in the framework have been performed successfully and promising results have been obtained. Moreover, we started with the scaled-up of the most suitable hybrid catalysts combining different accessible actives sites stabilized in the same network for performing reaction processes with industrial interest related with the production of commodities and platform pharmaceutical compounds. The use of suitable bi-functional organic-inorganic hybrid porous catalysts, combining base and redox active sites, have been used to carry out effectively consecutive tandem reactions based on aldolic condensations followed by hydrogenation processes to selectively obtain high added value products.

WP4 – Characterisation of materials and computational studies

The hybrid catalysts have been physico-chemically characterised. Additionally, the nature and accessibility of the active sites has been studied.

WP5 – Laboratory validation of hybrid catalysts

Test protocols for the asymmetric catalysis have been established and a preliminary evaluation performed. A structure-property correlation for Suzuki and tandem reactions has been carried out and the catalytic outputs have been optimised for fine-chemical and pharma applications, and the post-catalysis characterisation has been performed.

Moreover, the catalytic evaluation of hybrid catalysts in processes with relevant interest as proof-of-concept, showing the potentiality of the catalytic systems have been performed. In particular, for Suzuki-Miyaura or aldolization catalytic processes and combination of them.

WP6 – Catalytic reactions with direct application in the formulation of speciality chemicals

The catalytic evaluation of hybrid catalysts in processes with relevant interest to perform reaction processes with interesting application for the production of commodities or high added-value products have been studied. Especially for tandem onepot reactions based on furfural conversion followed by hydrogenation processes.

WP7- Catalytic reactions with direct application in the formulation of pharmaceutical compounds

Catalytic evaluation of hybrid catalysts in processes with relevant interest to perform reaction processes with interesting application in pharmaceutical field. In particular, for Suzuki-Miyaura or Friedel-Krafts reaction processes.

WP8 – Industrial validation and LCA

The two-stage model-development strategy has been successfully applied to model the targeted catalytic synthesis in the batch-type reactors, firstly Furfural-MIBK aldol condensation, and then both Furfural-MIBK aldol condensation and adduct hydrogenation. According to the parameter estimation result, it can be concluded that the commercial catalyst (i.e. Pd/Al₂O₃) is more active for both aldol condensation and hydrogenation, the targeted hydrogenation product (i.e. HMF) is less promoted, whereas, the novel catalyst is more selective for HMF.

The performances of the bi-functional catalysts were successfully evaluated for the two-step cascade synthesis (i.e. furfural-MIBK condensation + adduct hydrogenation) in a gas/solid/liquid fixed bed reactor.

A Life Cycle Assessment (LCA) of a pharmaceutical building block obtained by a Suzuki coupling reaction involving Pd-NHC-Silica was carried out and compared to the same reaction catalysed by the commercial tetrakis(triphenylphosphine)-palladium Pd(PPh₃)₄. This comparative study provides information on the potential gain of the new multi-site organic-inorganic hybrid catalysts as well as key levers for reducing environmental impacts of the targeted product

WP9 – Dissemination and exploitation

Exploitation activities – Industrial workshop at FEZA conference: cancelled

In order to engage the different stakeholders even more in the project, an industrial workshop was planned for 2020. All partners agreed that the most effective way to achieve maximum impact and engagement was to combine the Industrial Workshop with a relevant conference. After considering various possible conferences, the consortium decided to organise the Industrial Workshop together with the FEZA Conference (Brighton, UK, 12-15 July 2020).

In fact, everything had already been agreed with the organisers of FEZA, the workshop planned, and different sessions prepared. But then the conference unfortunately had to be cancelled by the organisers due to the pandemic. At first, the consortium had decided to postpone the event to autumn when the situation would have improved, however, the situation had not eased enough. As most conferences are still not taking place, we had to decide to cancel the industrial workshop completely.

Dissemination activities

The MUTI2HYCAT consortium published 3 more scientific publications related to the preparation, characterisation, modelling and application of hybrid catalysts. In total, 17 publications have been issued during the project so far, while the original goal was 6. Due to the pandemic, almost all congresses/conferences were cancelled or only held virtually, which was also due to travel restrictions in many countries. ITQ participated in one virtual conference.

Articles

• The significance of metal coordination in imidazole-functionalized metal organic frameworks for carbon dioxide utilization

William R. Webb Matthew E. Potter Daniel J. Stewart Stuart J. Elliott Pier J. A. Sazio Zhongxing Zhang He-Kuan Luo Jinghua Teng Liling Zhang Chiara Ivaldi Ivana Miletto Enrica Gianotti Prof. Robert Raja, Chemistry - A European Journal, 2020, 60, 13606-13610; https://doi.org/10.1002/chem.202001561

- A smart use of biomass derivatives to template an ad hoc hierarchical SAPO-5 acid catalyst
 Francesco Mariatti, Ivana Miletto, Geo Paul, Leonardo Marchese, Silvia Tabasso, Maela Manzoli,
 Giancarlo Cravotto and Enrica Gianotti, RSC Adv., 2020,10, 38578-38582,
 https://doi.org/10.1039/D0RA06353C
- Probing the Design Rationale of a High-Performing Faujasitic Zeotype Engineered to have Hierarchical Porosity and Moderated Acidity

Dr. Stephanie Chapman Dr. Marina Carravetta Dr. Ivana Miletto Dr. Cara M. Doherty Hannah Dixon Dr. James D. Taylor Prof. Enrica Gianotti Prof. Jihong Yu Prof. Robert Raja; *Angewandte Chemie International Edition, Volume 59, Issue 44 p. 19561-19569* https://doi.org/10.1002/anie.202005108

Conferences

Organic-Inorganic Hybrid Materials: From Random to Specific Location of Active Sites, 27 May
 2020 , Virtual meeting; ITQ (Dr. Urbano Díaz): https://www.youngcatalysis.net/

Upcoming events

Below you will find a list of future interesting events which also might be attended by the MULTI2HYCAT partners. Some of them will be held virtually.

- Global Conference on Catalysis & Applied Chemical Engineering, 23 25 April 2021 (Dubai, United Arab Emirates)
- 7th Edition of International Conference on Catalysis, Chemical Engineering and Technology, 17-18 May 2021 (Tokyo, Japan)
- 4th World Congress & Expo on Chemical Engineering and Catalysis, 14-16 June 2021 (Osaka, Japan)
- **★** FEZA conference, 5-9 July 2021 (Online)
- The Curious2021 Future Insight Conference, 12-14 July 2021 (Online)
- **★** ECCE13 & ECAB6—13th European Congress of Chemical Engineering & 6th European Congress on Applied Biotechnology, 19-23 September 2021 (Online)
- CAT2021, 27-29 September 2021 (Paris, France)
- 9th Edition of International Conference on Catalysis, Chemical Engineering and Technology, 21-23 October 2021 Orlando (USA)
- ♣ 2nd International Conference and Exhibition on Chemical Engineering & Catalysis, 25-27
 October 2021 (Cologne, Germany)
- Global Summit on Catalysis, Chemical Engineering and Technology, 8-10 November 2021 (Marseille, France)
- International Conference on Chemical Engineering and Heterogeneous Catalysis, 18-19 November 2021 (Paris, France)
- Chemspec Europe, 29-30 September 2021 (Frankfurt, Germany)

This is only a preliminary list for 2021. Visit the event section of our website regularly and find out more about the type, the titles and our people presenting at the different events!

Stakeholder Engagement – Participate in our Online Survey

In order to involve industrial and academic stakeholders from outside, the MUTI2HYCAT consortium launched an online stakeholder survey last year. The stakeholder online survey can be found on the project website.

Please participate in our online survey since your personal opinion is important for us! Based on your answers, we want to identify the innovation potential for the chemical industry on the one hand and better meet your expectations on the other hand.

This survey should not take longer than 10 minutes. Thank you for granting us your time!

Contact Us

You can't make it to the events? Do you have ideas or want to partner with us? Are you interested in details or have questions? Whatever you desire, you can contact us at any time using one of the channels below. Looking forward to your message and your participation in our survey!



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For more info about the project visit the MULTI2HYCAT website at: www.multi2hycat.eu ADMULTI2HYCAT





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