



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

### Enjoy Reading our First Biannual MULTI2HYCAT Newsletter in 2019

Welcome to our first biannual newsletter in 2019 where we inform you about the progress and MULTI2HYCAT achievements made in the last 6 months (Q3/Q4 2018) and give an outlook to the upcoming six-month period.

### SUMMARY AND HIGHLIGHTS

- **5<sup>th</sup> biannual project meeting held in Dresden (Germany) in December 2018.**

The 5th biannual MULTI2HYCAT project meeting was hosted by PNO and held after 24 project months in Dresden. The consortium discussed the latest achievements and the recommendations of the EU Expert.

- **Over 50 MULTI2HYCAT catalysts based on acidic, basic and metallic sites have been developed including the first real multi-site organic precursors.**

During the past 24 months, the partners have synthesized over 50 catalysts and assessed their material and catalytic properties and probed their effectiveness in several distinct reactions.

- **11<sup>th</sup> scientific article published in January 2019.**

The project results have been disseminated into 5 new publications within the last 6 months. These articles are focused on several MULTI2HYCAT topics ranging from preparation methods to rational characterization and computational studies.

- **11 oral presentations and 3 posters at 8 conferences.**

- **6 deliverables uploaded to the EU Participants Portal and another 2 milestones reached.**

- **Stakeholder Online Survey is still online. First results published confidentially to the EU.**

To engage with the specialist audience outside the MULTI2HYCAT consortium, we have designed a stakeholder survey and kindly invite you to tell us your opinion about the project, the approach and collaboration potential.

- **Read more recent scientific publications on the topic of "Hybrid Catalysts".**

Finally, we have looked up some recent articles related to our project. Check this section, if you are interested in the topic and like some cross-reading.

- **Feel free to [contact us](#) on any of the channels shown below, if you wish to collaborate or express your ideas or questions and check the [future events](#) which will be attended by MULTI2HYCAT partners and get into a personal discussion.**

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From December 13th to 14th 2018 the MULTI2HYCAT Consortium has met in Dresden to discuss the progress made during the previous 6 months. The main topics were the

- Preparation and characterisation of hierarchically porous catalysts prepared by unconventional bottom-up approaches.
- Modelling of novel materials and their catalytic properties, with a special emphasis of the design of molecular linkers for hybrid catalysts ensuring the most effective configuration.
- Influence of dactility and podality on the stability and activity of the active sites. Learn more about this topic by reading our [latest paper mentioned below](#).
- Activity, recyclability and stability under variable reaction conditions.
- Methodology of Techno-Economical and Life-Cycle Assessments and obtained results.

The development of the multi-site catalysts, their evaluation in the synthesis of speciality chemicals and pharmaceuticals as well as their LCA are crucial to unravel the exploitation potential of the project outcomes and their contribution to innovation and the European and global markets.

Promising results have been obtained in terms of catalyst development and reaction engineering. Now, the consortium is focussing on the preparation and catalytic testing of the multi-site materials. This includes:

- Selecting the top-performing catalysts,
- Developing catalytic protocols for multi-step reactions and, consequently,
- Combining active sites to obtain the desired multi-site catalysts.

So far, we are in line with our ambitious time plan. We have uploaded 6 new deliverables to the EU Participants Portal for evaluation and have reached two further milestones.

Our next biannual meeting will be hosted by Prof. Robert Raja and will be held in Southampton.



**5th MULTI2HYCAT Consortium Meeting**

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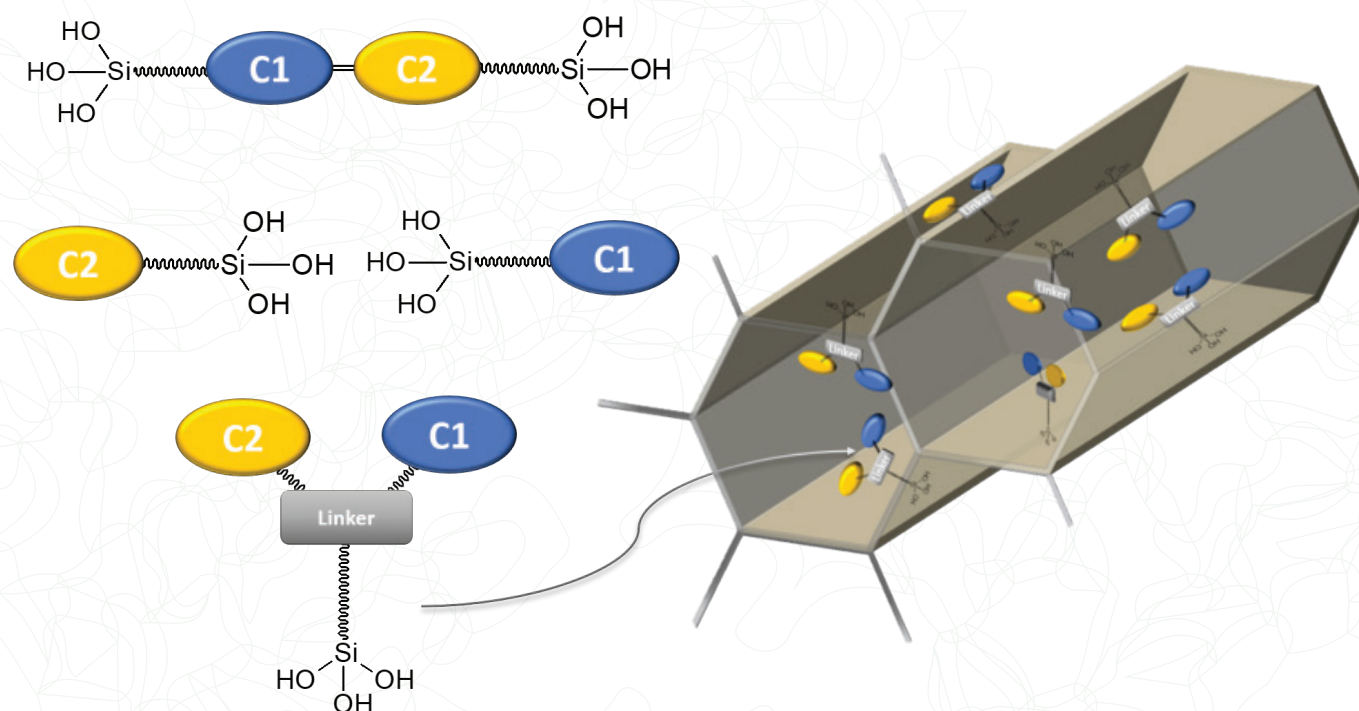


The envisaged organic-inorganic hybrid catalysts consist of the inorganic nanoporous support, mainly zeolites and zeotypes, and an organic or metal-organic structure, which can be located within the pore walls or protrude from the walls into the pores as sketched in the figure below (right). The inorganic support usually comes with an acid and/or size-selective functionality, where typical materials are ZSM-5, MCM-41 or 48, SAPOs and ALPOs. To obtain more space for the organic part of the hybrid catalysts, we create hierarchical porosity. The organic functionalities are manifold and based on typical catalysts applied in homogeneous catalysis. Our current focus lies on:

- Arylsulfonic acids for Friedel-Crafts Acylation,
- Basic amine and ammonium catalysts for Knoevenagel Condensations, Aldol Condensations and Michael Reactions,
- Metal-based catalysts for Suzuki-Miyaura Couplings and aligned to the main objective of the project,
- Multi-site catalysts based on the above-mentioned.

The left side of the picture below shows three general structural schematics to facilitate the heterogenization of the organic sites (S1 and S2), where the upper structure, so-called bridged silsesquioxanes, create the organic functionalities inside the catalyst walls and the middle and lower structures allow the introduction of the active sites onto the pore walls, thus, protruding into the pores.

One can imagine a lot of combination of sites, as well as a cross-condensation of the structures below, thus, e.g., generating functionalities both in and on the walls. However, what looks easy on paper is tough in reality. Not only that the materials have to be prepared, but their activities and selectivities must be assessed for reactions with several substrates and recyclability, stability and regeneration may pose problems. To address these challenges, the MULTI2HYCAT consortium is built of material scientists, computational scientists, reaction engineers and experts in bio-based and pharmaceutical chemistry, who have prepared over 50 unique catalysts and tested them in hundreds of reactions.



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## ARTICLES, TALKS AND POSTERS IN THE PAST PERIOD

Since the release last newsletter in summer 2018 the MUTI2HYCAT consortium has published another 5 scientific publications related to the preparation, characterisation, modelling and application of hybrid catalysts.

Further, the partners attended 8 international conferences and summer schools, where they presented the latest project results in 11 talks and 3 posters.

### Articles

- Influence of Silicodactyly in the Preparation of Hybrid Materials
- Synthesis of 2D and 3D MOFs with Tuneable Lewis Acidity from Preformed 1D Hybrid Sub-Domains
- In Situ FT-IR Characterization of CuZnZr/Ferrierite Hybrid Catalysts for One-Pot CO<sub>2</sub>-to-DME Conversion
- Elucidation of the Interaction Mechanism between Organic Chiral Cages with Biomolecules through Nuclear Magnetic Resonance and Theoretical Studies
- Chiral Hybrid Materials Based on Pyrrolidine Building Units to Perform Asymmetric Michael Additions with High Stereocontrol

### Talks

- **"Multidisciplinary Approach for the Physico-Chemical Characterisation of Porous and Hybrid Materials"**, L. Marchese (UPO), Tutorial Talk at the 1st MULTI2HYCAT Summer School
- **"The Journey of a Medicine: From Invention to the Market"**, M. Crespo (Almirall), Tutorial Talk at the 1st MULTI2HYCAT Summer School
- **"Catalysis with Functional Porous Architectures"**, R. Raja (UoS), Tutorial Talk at the 1st MULTI2HYCAT Summer School
- **"Computational Techniques for the Characterisation of Porous Materials"**, M. Cossi (UPO), Tutorial Talk at the 1st MULTI2HYCAT Summer School
- **"Creating Hierarchical Silicoaluminophosphates with Tailored Acid Sites using Bottom-Up Synthetic Strategies"**, C. Ivaldi et al. (UPO), Talk at the 1st MULTI2HYCAT Summer School
- **"Chiral Non-Ordered Mesoporous Hybrid Catalyst to Enantioselective Michael Addition"**, S. Llopis et al. (ITQ-CSIC), Talk at the 1st MULTI2HYCAT Summer School
- **"Accessible Acid Sites in Hierarchical Architectures for Beckmann Rearrangement"**, E. Gianotti et al. (UPO / UoS), Talk at the XX Congresso Nazionale di Catalisi e XX Congresso Nazionale della Divisione di Chimica Industriale
- **"Recyclable Stereoselective Heterogeneous Secondary Amine Organocatalysts for Enal Activation"**, M. Meazza et al. (UoS), Talk at the American Chemical Society National Meeting & Exposition: Nanoscience, Nanotechnology and Beyond
- **"Reaccion de acoplamiento Suzuki-Miyaura para la obtención de biarilos de interés en la industria farmacéutica"**, M.C. Hernández Soto (ITQ-CSIC), Talk at the CICAT2018
- **"Organosiliceous Hybrid Base Catalysts – Synthesis and Reactivity"**, A. Erigoni et al. (ITQ-CSIC), Talk at the EFCATSSchool on Catalysis
- **"Preclinical Research Collaborations in the Pharmaceutical Industry: incentives and barriers"**, M. Crespo (ALM), Talk at the BioSpain 2018 Drug Discovery Pharma Biotech Forum

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## Posters

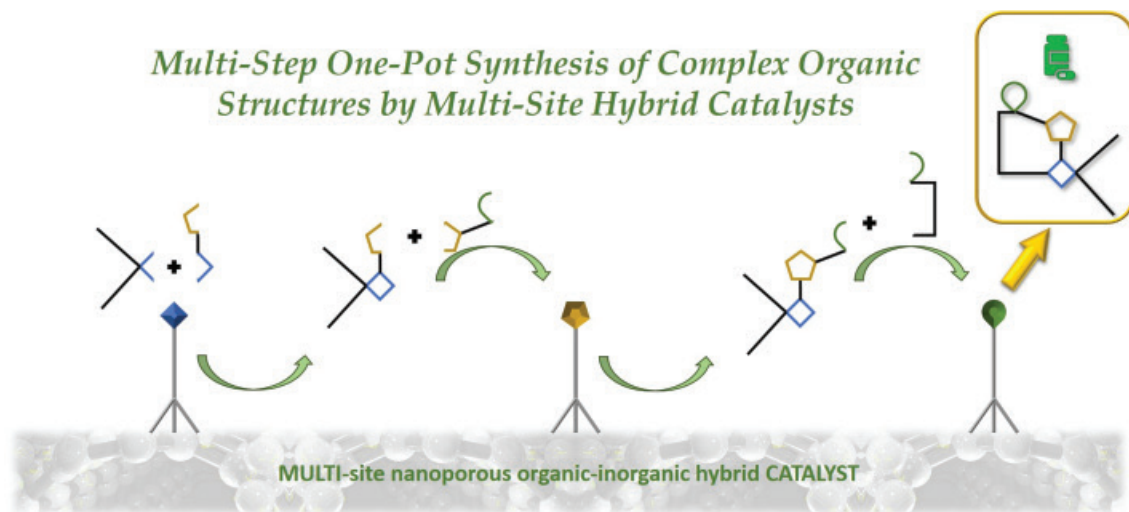
- **"Sustainable saccharide templates to drive the formation of hierarchical SAPO-34 with tunable acid properties"**, C. Ivaldi et al. (UPO / UoS), Poster at the Workshop Advanced Inorganic Materials: Green and Unconventional Synthesis Approaches and Functional Assessment
- **"Highly active mesoporous silica-supported base catalysts for C-C bond formation"**, C. Segarra et al. (ITQ-CSIC), Poster at the 6th International Conference on Multifunctional, Hybrid and Nanomaterials
- **"Hybrid acid catalysts: Synthesis and spectroscopic characterization"**, Andrea Erigoni et al. (ITQ-CSIC / UPO), Poster at the 6th International Conference on Multifunctional, Hybrid and Nanomaterials

## STAKEHOLDER ENGAGEMENT – PARTICIPATE IN OUR ONLINE SURVEY

Besides the Summer School, which was organized by ITQ-CSIC and held in 2018 at the Instituto de Tecnología Química in Valencia, the MULTI2HYCAT partners also intend to engage industrial and academic stakeholders from outside the consortium. To this end PNO prepared a stakeholder online survey in agreement with the other project partners. This stakeholder online survey has been published on the project website and has been promoted throughout our available communication channels. Further, over 130 invitations have been expressed to stakeholder from industry and academia. However, this is not enough to achieve the impact we wish.

We value your opinion about our project and, herewith, invite you to participate in our online survey.

## MULTI2HYCAT STAKEHOLDER ONLINE SURVEY



**Visit our website, take the survey and let us find out how you could benefit from the MULTI2HYCAT project!**

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## MULTI2HYCAT-RELATED PUBLICATIONS

For this section we have looked up some recent scientific articles related to the MULTI2HYCAT project

- [Heterogenized Ionic-Liquid Metal-Oxide Hybrids: Enhanced Catalytic Activity in the Liquid-Phase Beckmann Rearrangement](#)
- [Functional Acid and Base Hybrid Catalysts Organized by Associated \(Organo\)aluminosilicate Layers for C–C Bond Forming Reactions and Tandem Processes](#)
- [New Insights into Aldol Reactions of Methyl Isocyanoacetate Catalyzed by Heterogenized Homogeneous Catalysts](#)
- [Utilization of Waste Biomass for the Synthesis of Functionalizable Support for Covalent Anchoring of Active OrganoCatalyst.](#)

If you are interested in knowing more about MULTI2HCAT, the partners and our vision: [Contact us!](#)

## MEET MULTI2HCAT

Whether in research or in business, the best way to get in contact is having a personal and individual discussion with the experts. Below we list some conferences and fairs where you can interact with MULTI2HYCAT partners, ask your questions and learn more about our project. You can meet our leading scientists at:

- [British Zeolite Meeting](#) (11th – 12th April 2019, Birmingham, United Kingdom)
- [EUROPACAT 2019](#) (18th – 23rd August 2019, Aachen, Germany)
- [International Zeolite Conference IZC 2019](#) (07th – 12th July 2019, Perth, Australia)
- [Meeting of Young Researchers of the Real Spanish Society of Chemistry](#) (26th – 30th May 2019, Donostia-San Sebastián, Spain)

This is only a preliminary list for 2019. 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!

## 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!

[www.multi2hycat.eu](http://www.multi2hycat.eu) | [info@multi2hycat.eu](mailto:info@multi2hycat.eu)

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For more info about the project visit the MULTI2HYCAT website at: [www.multi2hycat.eu](http://www.multi2hycat.eu)  **MULTI2HYCAT**



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