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Bifunctional Zeolite based Catalysts and
Innovative process for Sustainable
Hydrocarbon Transformation GRANT
AGREEMENT N°: 814671

NEWSLETTER Nr. 4

20th December 2020



WHAT'S NEW?

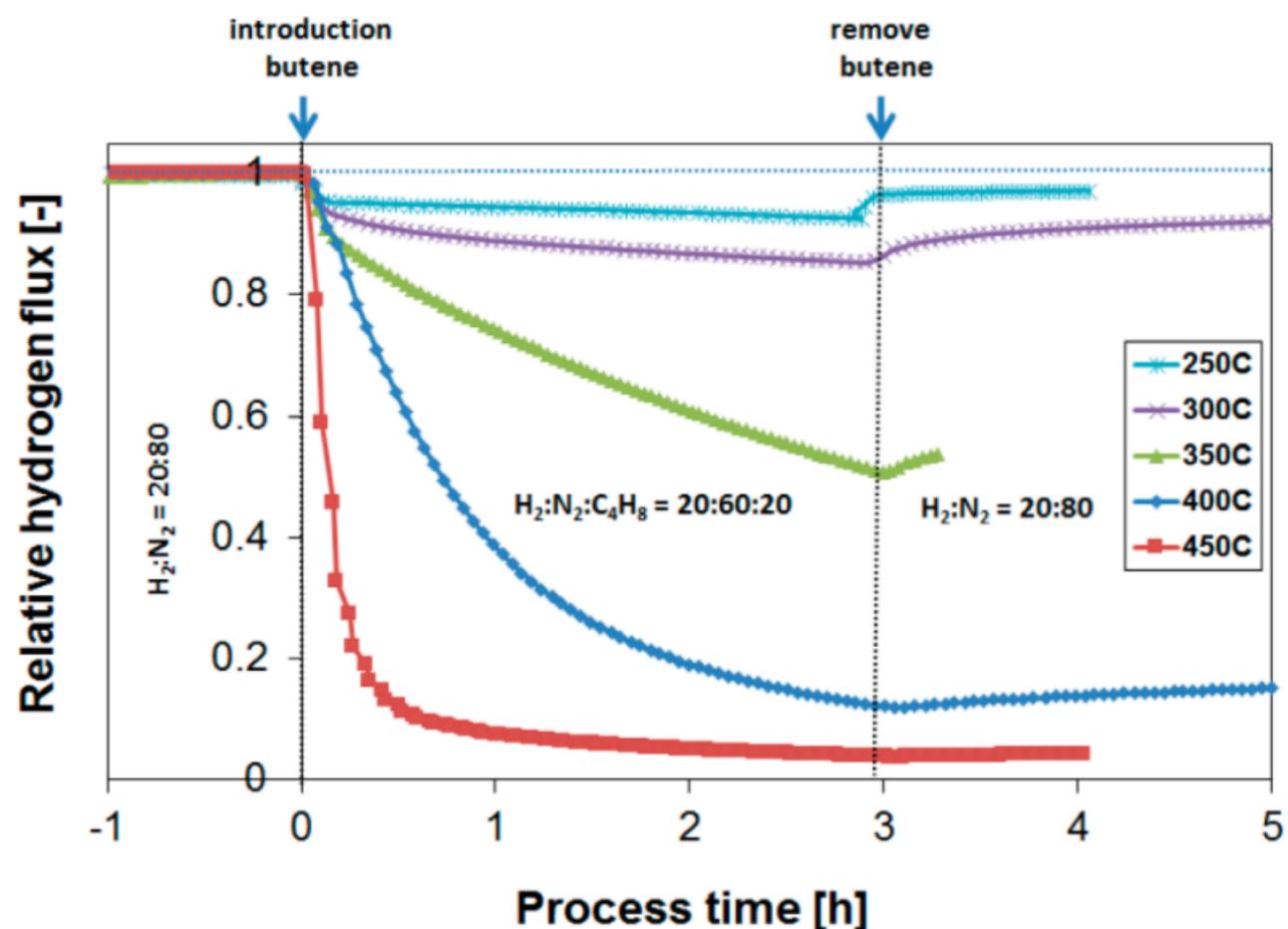
Due to the **COVID – 19** emergency several research activities have been delayed, nevertheless, in respect of the planned work, **BiZeolCat** Project is glad to inform you about the main results achieved so far. A plan for boosting activities has been put into practice to recover the delay in the next months.

Hoping this extraordinary situation will recover soon, BiZeolCat people recommend you stay safe and enjoy the newsletter reading!

Flux-Reducing Tendency of Pd-Based Membranes Employed in Butane Dehydrogenation Processes

Thijs A. Peters, Marit Stange and Rune Bredesen

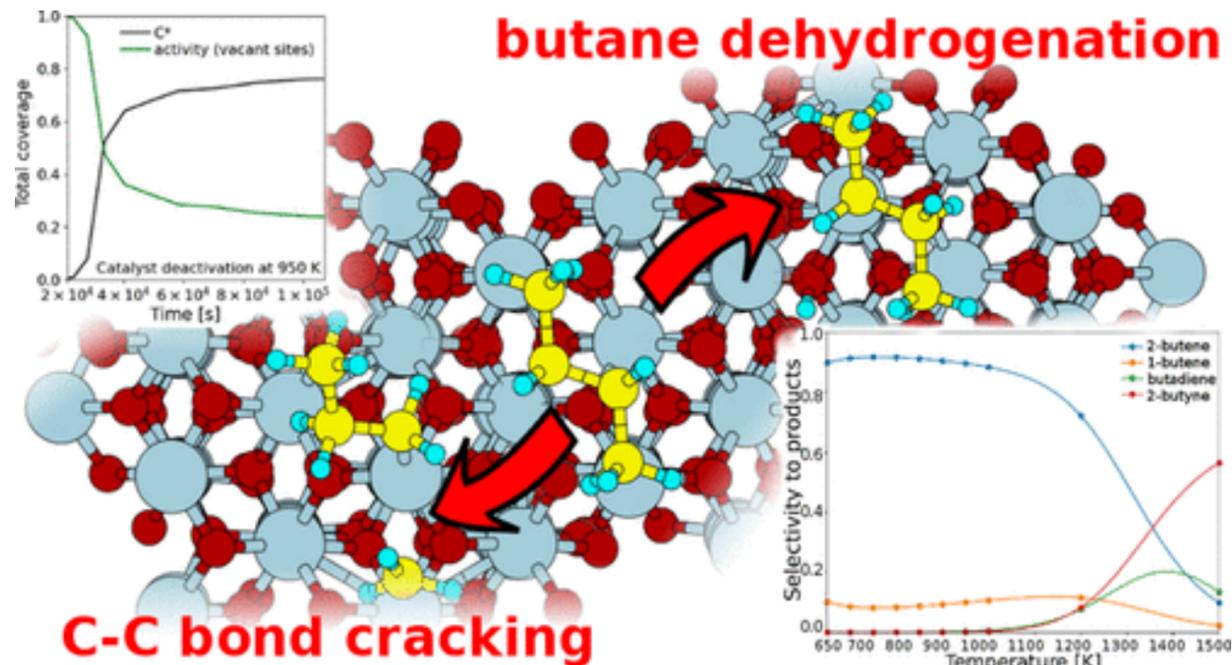
Alkene production by the catalytic dehydrogenation of light alkanes is an alternative to conventional heavy hydrocarbon cracking. Dehydrogenation is an endothermic equilibrium-limited reaction and is typically performed at elevated temperatures at close to atmospheric pressure. Even at 500 °C, the thermodynamic equilibrium conversion for propane dehydrogenation is less than 20%.



Further, the high operating temperature results in large amounts of carbon deposition on the catalyst, which implies the need for a periodic regeneration of the catalytic bed, leading to a complex plant design. Due to the removal of hydrogen from the reaction, membrane reactors have the potential to provide the same conversion and yield of a conventional process while operating at milder conditions. In the study, a wide range of operating conditions, such as temperature (200–450 °C) and H₂/butylene (or butane) ratio (0.5–3), on the flux-reducing tendency were investigated: an optimal performance was found at 250–300 °C for obtaining the highest absolute hydrogen flux in the presence of butylene. At lower temperatures, the competitive adsorption of butylene over hydrogen accounts for a large initial flux penalty.

Open Access manuscript: doi.org/10.3390/membranes10100291

**First-Principles-Based Multiscale Modelling of
Nonoxidative Butane Dehydrogenation on
Cr₂O₃(0001)**



Drejc Kopač, Damjan Lašič Jurković, Blaž Likozar and Matej Huš

Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry (Slovenia)

Propane and butane are short straight-chain alkane molecules that are difficult to convert catalytically. Analogous to propane, butane can be dehydrogenated to butenes (also known as butylenes) or butadiene, which are used industrially as raw materials when synthesizing various chemicals (plastics, rubbers, etc.).

In this study, we present results of detailed first-principles-based multiscale modelling of butane dehydrogenation, which can be paralleled to experimental data.

We found that among all the dehydrogenation products 2-butene ($\text{CH}_3\text{CHCHCH}_3$) is the most abundant product of dehydrogenation, with selectivity above 90%, concluding that the dehydrogenation of butane is a viable alternative to conventional olefin production processes.

Enjoy the full reading: pubs.acs.org/doi/10.1021/acscatal.0c03197

Website: BiZeolCat Informs!

New in the website [#BiZeolcatInforms!](#) is born to present the assumptions on which the project's scopes rely on to the general public. BiZeolcat, even facing high technological issues, aims to have huge impacts on the whole society, fostering circular economy and helping the economy's decarbonization. Therefore the general public is one of the most important stakeholders of the project.

Thanks to short notes reporting information about the main topics (chemistry, physic, Industrial processes) involved in the project development, BiZeolcatInforms! aims to reduce the gap in communicating the project's impacts on the wider audience possible.

BiZeolCat People

Oleg Pajalic - PERSTORP

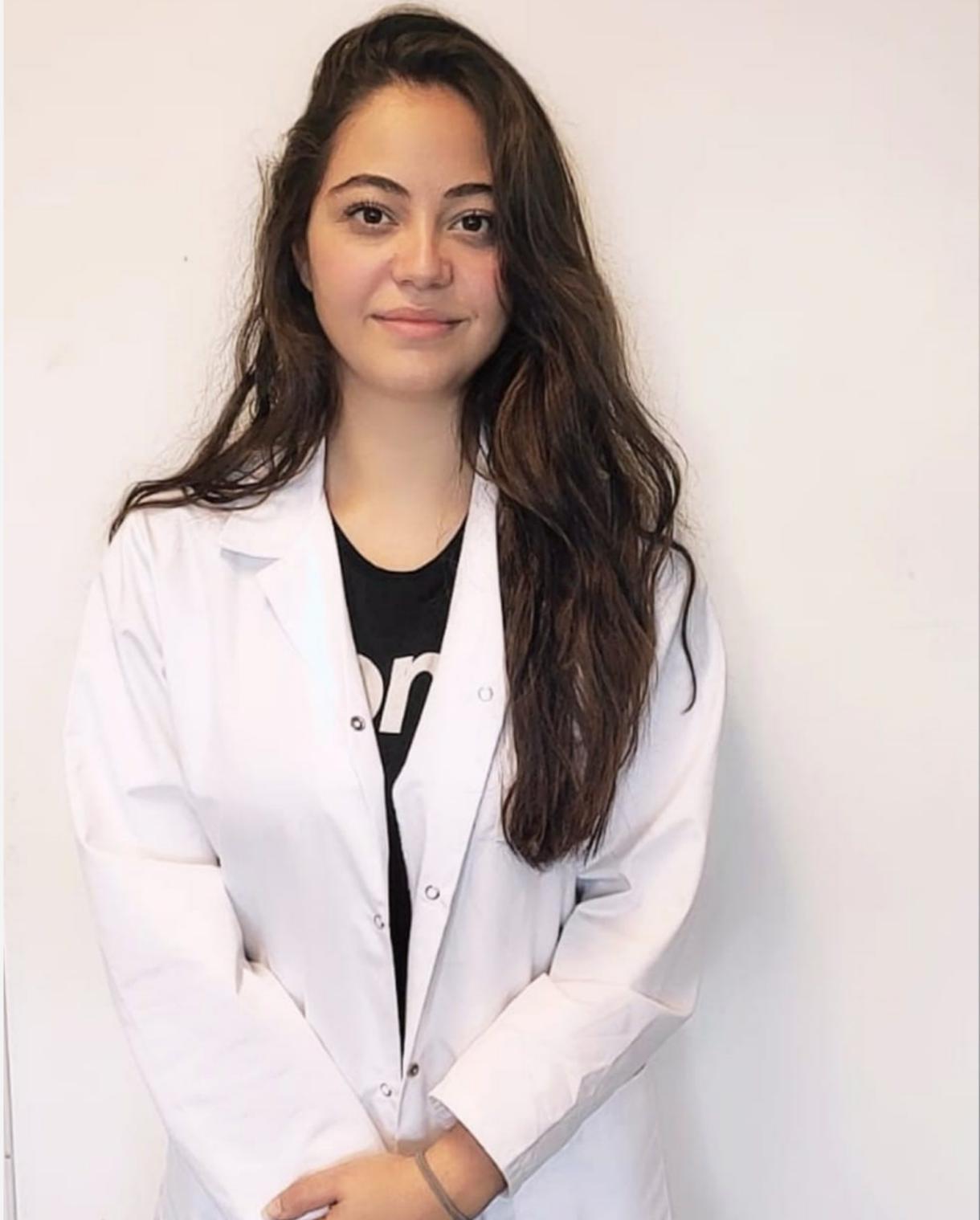
(Picture kindly by Ines Sebalj)



Perstorp role in the project is to evaluate olefins, produced by the new catalytic technology to be developed in BIZEOLCAT, in pilot hydroformylations unit. My role in the project is to coordinate the project from Perstorp side.

The major goal towards green economy is to remove net emissions of CO₂ and GHG and in it is line with Perstorp strategy to support innovative activities helping reaching the goal. BIZEOLCAT will develop new, more efficient catalyst which is in my opinion the key activity on the way forward as more selective, efficient and milder synthesis and that will reduce both waste and energy use. The catalyst research in BIZEOLCAT may also contribute to developing an efficient olefin synthesis which will be based on sustainable raw materials in near future.

Jessy Abou Nakad – CPE Lyon CNRS



My name is Jessy ABOU NAKAD and I am a PhD student in C2P2-CNRS in Lyon. I am actively involved in WP2 and WP3, comprising preparation and characterization of innovative single sites catalysts on classical oxide and meso-zeolites for the applications in important reactions in petrochemistry such as propane and butane/butenes dehydrogenation and propane aromatization. These new catalysts are prepared through surface organometallic chemistry approach by a judicious choice of organometallic precursors and support based on the elementary step of the mechanism of these desired reactions. Preliminary catalytic performances of the catalysts are also investigated in continuous flow reactor in CNRS. The best catalysts are sent to SINTEF for high throughput testing.

The surface organometallic approach allows access to isolated metal-sites being decorated in support materials. As the targeted reactions involve a dehydrogenation step, and recent studies strongly suggest that the active site is isolated, the innovative catalysts are expected to contain 100% active sites on the surface. The latter will have several impacts:

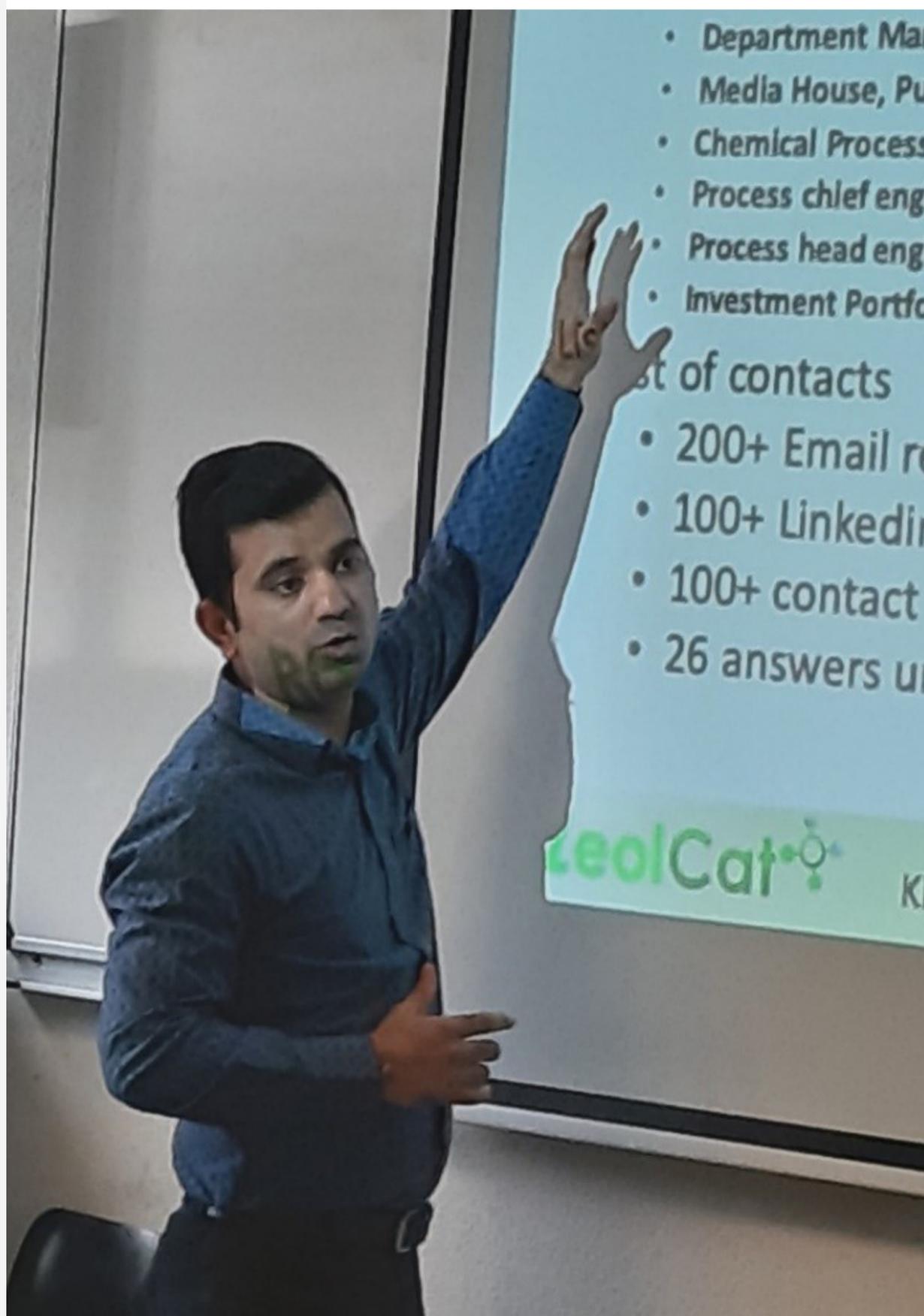
- ⑥ Reduce the metal loading of the heterogeneous catalysts, resulting in a reduce in the price and the amount of the catalyst when keeping the high catalytic performance,

improving the atom economy of the catalysts, generate less waste and reduce the environmental impact

- ⑥ As the nature of the targeted catalysts is heterogeneous and similar to the existing commercial catalysts, it is believed that the BIZEOLCAT catalysts may be easily adaptable with the existing infrastructures and thereby minimize the CAPEX.
- ⑥ A particular task in the project is to explore alternative elements to replace the commercial chromium catalyst which needs a high loading of metal around 20 wtCr%. This will significantly reduce human and environmental risks.

COVID-19 has resulted in the lockdown of the laboratory, being back to work in May 2020. Without access to the laboratory facilities, the experimental works were inevitably set to hold, resulting in a delay to the initial Gantt Chart. However, a plan was added to boost the activities and to minimize the impact of COVID on the project.

Mayur Soni – STRANE INNOVATION



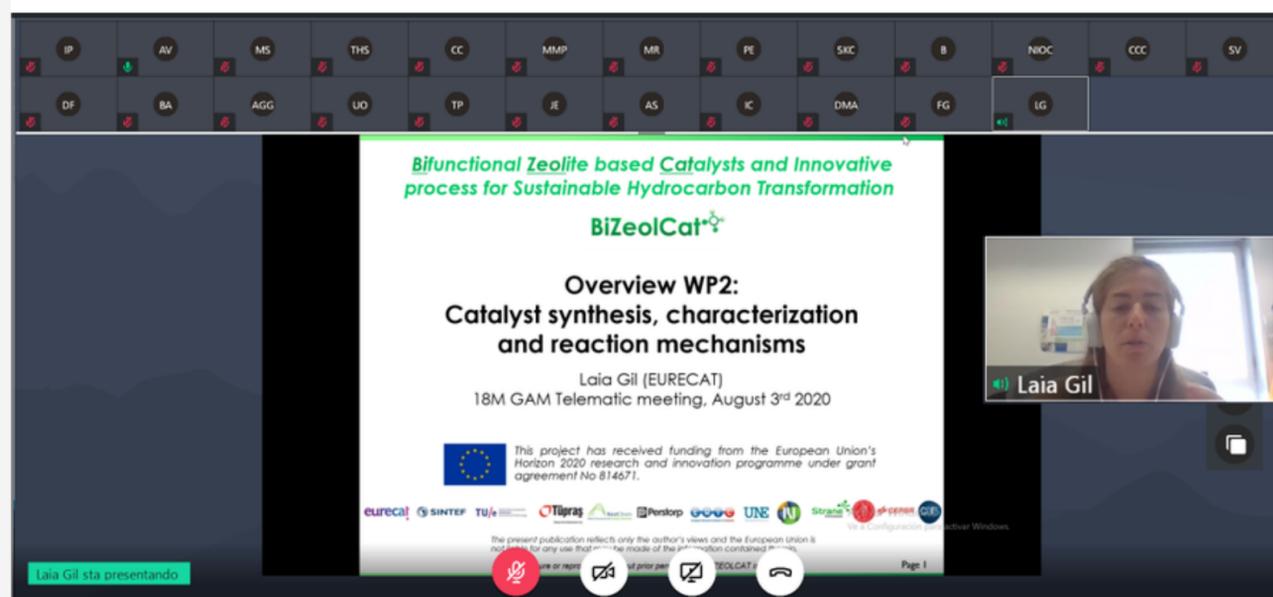
Strane Innovation is Participating as a Startup Studio, Who creates spin-off's out of innovative ideas and launch in the market. We are focusing on two main tasks in BIZEOLCAT project: one is Market analysis and the second one is Exploitation activities (Creation of a Startup or Joint venture).

BIZEOLCAT project will make a positive impact on the Refining and Petrochemical industry towards sustainability, Circular Economy and reduction in Green House emission, Since these industries are playing a major role in greenhouse gas emission, due high demand in petrochemical building blocks, which leads to increase in emission directly. With BIZEOLCAT project, industries will able to reduce their emission and carbon footprints to the environment with less consumption in energy and increase in production rate.

Due to COVID 19 situation, Refining and Petrochemical industries are stabilising their cash flow, Optimising their operations and Reimagining in their business portfolios, that will give a room to BIZEOLCAT technology to enter in the market.

BIZEOLCAT EVENTS

5th VIRTUAL GENERAL ASSEMBLY



Date 23rd June 2020

The main objectives of the meeting were the assessment of the project's achievements (milestones and deliverables) and a plan for the next steps. The meeting has been very intensive and all the participants collaborate actively providing a friendly atmosphere and strengthening the relationships among the partners filling the gap of being effectively remoted connected.

UNPRECEDENTED VIRTUAL FORUM

Fira Barcelona te invita al webinar

UNPRECEDENTED
VIRTUAL FORUM

UNPRECEDENTED VIRTUAL FORUM | Tech Transfer Forum

Martes, 17 de noviembre 2020 - 12:30 (CET) ▾

Aitor Gual Gozalbo from Eurecat - Technology Centre of Catalonia presented Bizeolcat Project at the UNPRECEDENTEDVirtualForum organized by Fira Barcelona within SemanaDeLaCiencia 2020 (Spain).

The UNPRECEDENTED Virtual Forum highlights the most advanced proposals for the development of Circular Economy and Digital Futures based on Technology Transfer.

Bizeolcat took part in the Tech Transfer Forum that aims to present innovative projects connecting companies with research groups and project funders.

The protagonist's sectors were Sustainable construction, Food, Energy, Mobility since they make up the priority sectors of the Circular Economy Action Plan. All the presented projects were in an advanced phase so that companies, scientists and the community could carry out the transfer.

UPCOMING EVENTS

5th VIRTUAL GENERAL ASSEMBLY

January 28th and 29th 2021

The main objectives of the meeting will be the assessment of the project's achievements (milestones and deliverables) and a plan for the next year.

All the details of the event will be reported on the project website just after the meeting close. STAY TUNED!

2021 Dissemination Activities

Several dissemination events were planned for the year 2020, however, due to the covid19 emergency, most of them have been cancelled and postponed to 2021 or even 2022.

Here the latest news on which are still in the Project dissemination plan for 2021.



International Symposium on Chemical Reaction Engineering (ISCRE26)

India – New Delhi - December 2021 Our Partner from National Institute of Chemistry (Slovenia) planned to present results on: Propane dehydrogenation on Cr₂O₃: kinetics and mechanism of the reaction and catalyst deactivation M. Huš, D. Kopač, B. Likozar

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Visit the **BIZEOLCAT** project at the address – www.bizeolcat.eu and follow the project on LinkedIn, Twitter and YouTube.

Let us have your comments!

The next issue of the Newsletter will be released in June 2020

Bizeolcat H2020 Project GRANT AGREEMENT N°: 814671
Company Address, Phone Number
Bizeolcat 2019

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