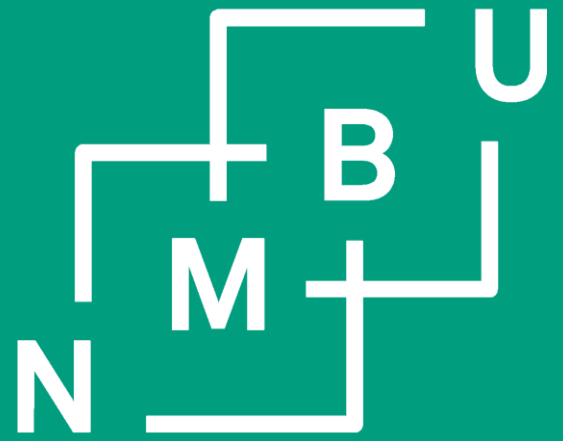
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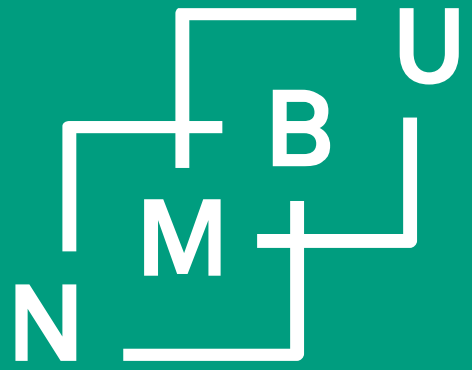


Norwegian University
of Life Sciences

Funded by the European Union

HORIZON-MSCA-2021-SE-01-01, project number 101086363

UNPRECEDENTED – Unrevealing the mechanism involved when producing biodiesel form waste oil using a combined experimental and theoretical methodology

Webinar: The 2023 call of MSCA Staff Exchanges

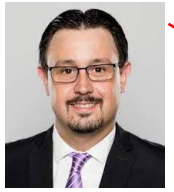
Professor Jorge Mario Marchetti - Physics Institute
Faculty of Science and Technology -Norwegian University of Life Science

November 28th 2023

Summary:

- 3 international parties
- 4 Year project (January 2023)
- Staff exchange among parties
- Lead by NMBU Norway

Norges miljø- og biovitenskapelige universitet



UNS UNIVERSIDAD NACIONAL DEL SUR

ISEL INSTITUTO SUPERIOR DE ENGENHARIA DE LISBOA

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Dr. Graciela Brizuela

Dr. Pablo Bechthold

Dr. Estela Pronsato

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Dr. Julian Juan

Dr. Alejandro Gonzalez Fa

Abstract *

40% reduction on emissions should be achieved by 2030 within EU with the outstanding goal for Europe to become the first climate neutral continent by 2050. These goals need to be reached without jeopardizing economic development and growth, and simultaneously fulfilling the UN goals for sustainability.

One of the main contributors to climate change and global warming is emissions from our vehicles as these mainly use petroleum-based fuels. To address this, new approaches, methodologies, and technologies must be developed.

Biodiesel is one option to substitute diesel; however, its production has been controversial since it requires the use of edible oils and thus creates conflicts with the production of food crops, making it less attractive. Because of this problem, newer technologies are being developed to treat lower quality nonedible oils. However, as yet, these are not economically viable.

To address these problems, UNPRECEDENTED will focus on the use of waste oil. This new raw material has been tested experimentally with promising results. However, how the reaction is taking place and the steps involved is far from being understood. This lack of knowledge has a negative effect when selecting new technologies or testing new feedstocks.

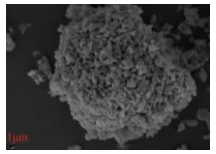
UNPRECEDENTED will use a combine methodology of experimental data and theoretical modelling (DFT based calculations) to study and fully comprehend the biodiesel production reaction. This methodology will permit a full understanding of the reactive steps involved, the reaction pathway that is followed as well as the energies involved in each reactive step. This methodology will assess for the conversion of waste oil in the presence of renewable alcohols to produce biodiesel when using new catalytic materials that are biobased, produce from renewable sources, and enriched with glycerol.

What do we do in UNPRECEDENTED?

Biomass

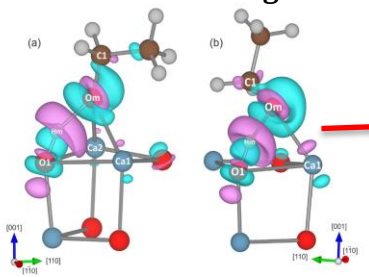
Catalyst preparation

Characterisation

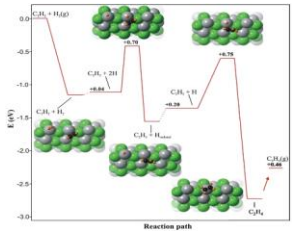


Enhancing through dual input approach

DFT modeling



Kinetics modeling

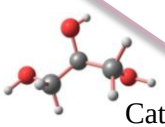


Biofuel

Feedstocks

Jojoba seeds

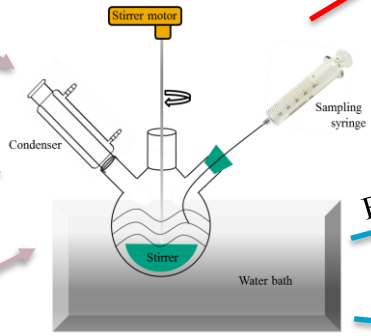
Algae



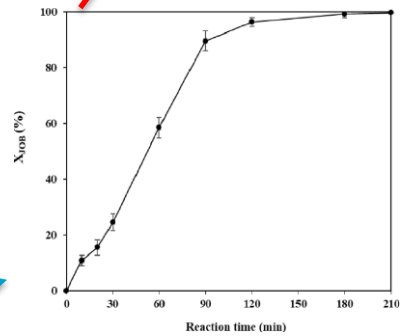
Catalysts Enrichment

Non-edible oil

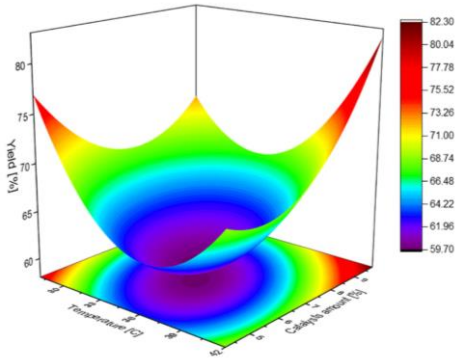
Renewable alcohol



Experimental data



Optimization work (DOE & RSM)



Bioproductss

Lubricants

Health

Cosmetics

Table 3: Work Package description

Work Package no.	1	Start/End month	1/48
Work Package title	Project Management		

Work Package no.	2	Start/End month	1/24
Work Package title	Preparation and characterization of the new catalysts		

Work Package no.	3	Start/End month	12/36
Work Package title	Experimental testing of catalysts and reaction optimization		

Work Package no.	4	Start/Eend month	12/48
Work Package title	Development models based on DFT calculations and kinetics		

Work Package no.	5	Start/End month	1/48
Work Package title	Education and training		

Work Package no.	6	Start/End month	1/48
Work Package title	Communication and dissemination of results		

Deliverables In detail

Deliverable	Months 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
Data management plan	
Dissemination and exploitation	
Conference 1	
Catalysts preparation	
Transfer of info	
Paper 1	
Progress report M13	
Mid term meeting	
Training course 1	
Conference 2 & 3	
Workshop 1	
Catalysts characterization	
Catalysts activity	
Catalysts enhacement	
Conference 4	
Paper 2 & 3	
Paper 4	
Sensitivity study	
Training Course 2	
Conference 5	
Conference 6	
Paper 5	
Optimization	
Glycerol enrichment	
Conference 7	
Paper 6	
Training Course 3	
Reaction energies	
Workshop 2	
Conference 8	
Kinetics	
Paper 7	
Project management	

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The adsorption of ethyl formate on CaO: A DFT study

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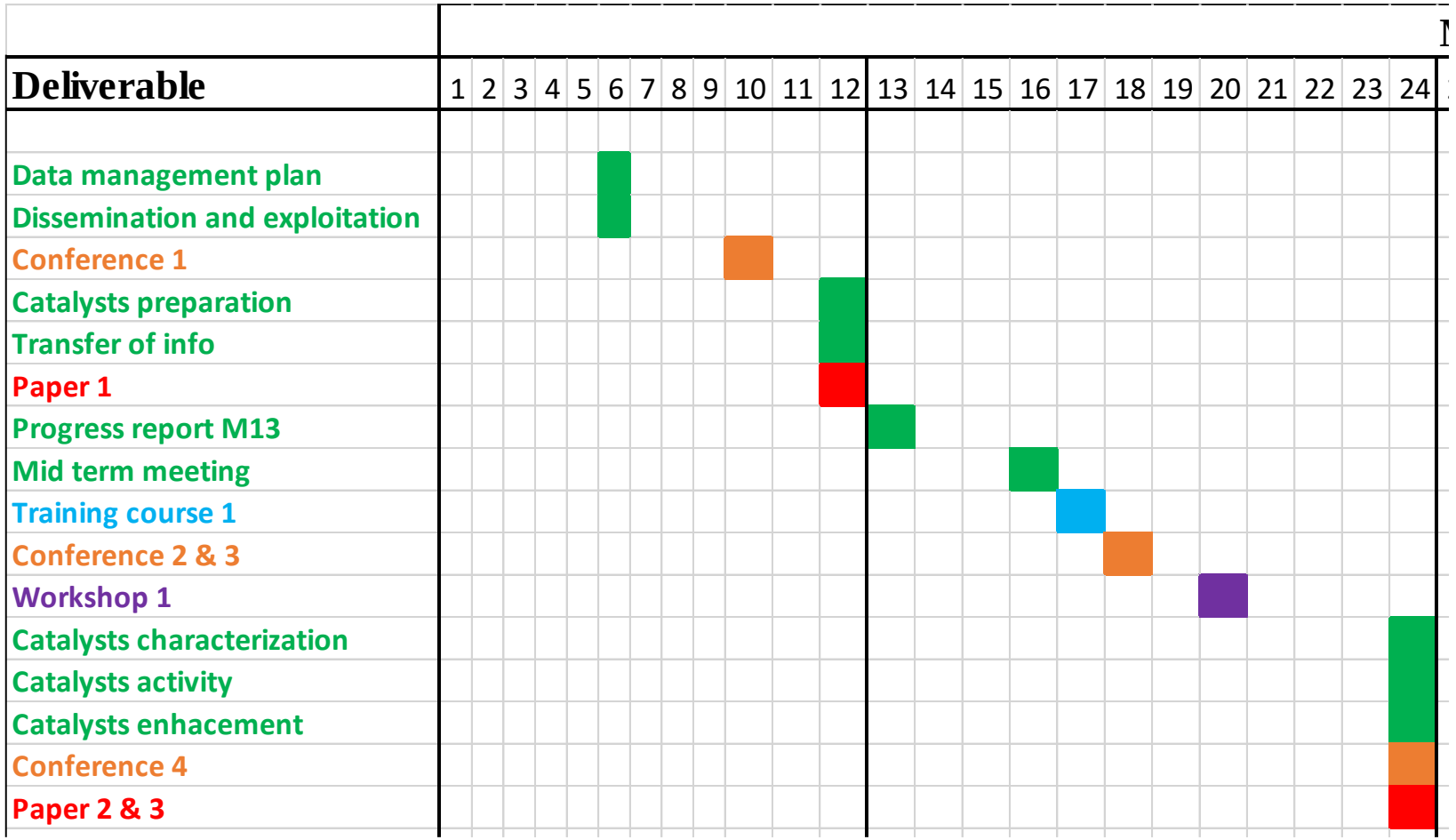
ARTICLE INFO

Keywords:
CaO
Catalyst
Ethyl formate
Adsorption
DFT

ABSTRACT

Ethyl formate adsorption on CaO (001) is analyzed using Density Functional Theory (DFT) with Van der Waals corrections, implemented through the Vienna ab Initio Simulation Package (VASP). Our calculations reveals a possible adsorption site at low coverage with adsorption energy of −1.21 eV, which is more stable than ethanol and less stable than formic acid. Both molecular oxygens bond to two Ca atoms and the C methyl bonds to a surface oxygen. The analysis of the electronic structure and bonding show a stabilization of ethyl formate as a result of a shift in its states to lower energies, with respect to the gas phase. A relaxed molecular geometry is obtained after adsorption with no dissociation detected. There is a charge transfer (0.20 e) from the adsorbate to the surface. At the same time, H–C (formate) experiences a charge decrease of 0.16 e. The Ca–O in the surface mostly shows a decrease in bond order after adsorption.

Period 1: 01/01/2023-31/12/2024

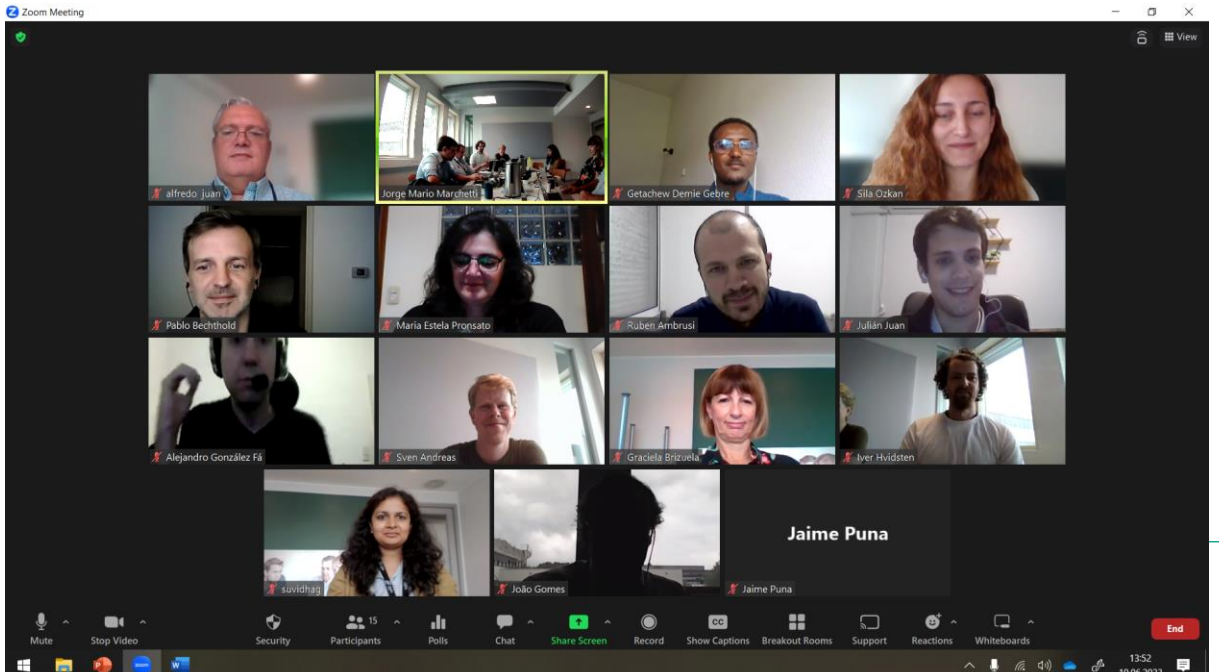


TRIPS

1. UNS to ISEL 4 PM
2. NMBU to ISEL 2 PM
3. UNS to NMBU 10 PM
4. ISEL to NMBU 3 PM

Benefits

1) Huge possibility for cooperation and joint research.
2) Budget for doing the secondments.
3) Opportunity for younger research career development.
4) Access to new facilities and new methodologies.
5) Involvement in a new research activity.



Challanges

1) High cost of living expenses in Norway, short secondments is not recommended.
2) Delays in the payment in receiving countries.
3) High taxes on transfer of budget and therefore lost of money.
4) Saving all traveling, financial information for 5 years after end of project.
5) Institutional numbers (PIC)

Thank you very much for your time