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## ZEOCAT – 3D: OVERVIEW AND MAIN GOALS

María Tripiana Serrano



## Basic project data

Title	Development of a bifunctional hierarchically structured zeolite based nano-catalyst using 3D-technology for direct conversion of methane into aromatic hydrocarbons via methane dehydroaromatization
Acronym	ZEOCAT-3D
Grant Agreement number	814548
Coordinator	OPTIMIZACION ORIENTADA A LA SOSTENIBILIDAD SL (IDENER)
Start date	1st of April 2019
End date	30th of September 2022
Overall Budget	€6,764,020
Eu Contribution	€6,764,020
Call	H2020-NMBP-ST-IND-2018
Topic	CE-NMBP-24-2018 - Catalytic transformation of hydrocarbons (RIA)

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# The context







Aromatics are esential for some of the most extensive petrochemical products



Their utilization is associated with severe environmental consequences (aquatic species destruction, global warming,..)



Current production methods are cosidered usustainable

### The context





Aromatics are esential for some of the most extensive petrochemical products



Their utilization is associated with severe environmental consequences (aquatic species destruction, global warming,..)



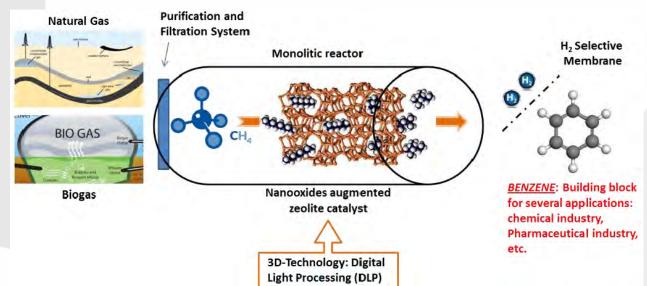
Current production methods are cosidered usustainable

The ZEOCAT-3D project proposes an alternative, which consists of obtaining these high-value chemicals (benzene, naphthalene, among others) from methane from sources like biogas and natural gas through an improved catalytic process called methane dehydroaromatization (MDA).





The goal of the project ZEOCAT-3D is the development of a new bi-functional (two types of active centers) structured catalysts, achieving for the first time a tetramodal pore size distribution (micro-, meso1-, meso2-, macro-porous) and high dispersion of metal active sites for the conversion of methane, coming from different sources as natural gas and biogas, into high value chemicals such as aromatics (benzene, naphthalene, among others) via methane dehydroaromatization (MDA).







Development and production of an improved catalyst



Design, construction and validation of a catalytic reactor



Rational design of catalyst / Multiscale modelling





Development and production of an improved catalyst



Design, construction and validation of a catalytic reactor



- ✓ Improved methane conversion (>50%)
- ✓ Increased selectivity towards benzene (>90%)
- ✓ Enhanced performance (7 times less deactivation)
- ✓ Higher yield rates (up to 80%)



Rational design of catalyst / Multiscale modelling



# Challenges and solutions



### Challenges and solutions

# Challenges of the MDA process

Difficult activation of the C-H bond of CH4 molecule, high reactivity of the products compared to methane, and acid sites of zeolites are occupied by coke deposition.

### Problems to solve

The main drawbacks associated the process are low methane conversion, low selectivity towards the desired products and the quick deactivation due to carbon deposition onto the catalyst.

### The solution

These problems will be overcome by the use of hierarchical zeolites structures synthesized by 3D-printing and loaded with doped molybdenum nanooxides.

### Challenges and solutions (Key elements)



### Catalyst

Development and production of improved catalyst, a 3D hierarchical structure with bi-functional activity (two types of active centers).

#### Reactor

Design, construction and validation of catalytic reactor, with improved productivity for direct methane MDA into aromatics.

### Modelling

Rational design of catalyst/multi-scale modelling, for achieving multimodal pore size distribution (micro-, meso1-, meso2-, macro-porous).

#### Feedstock

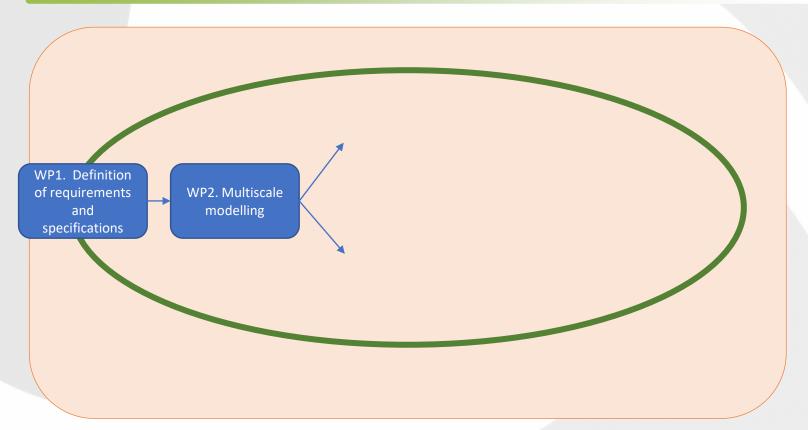
Optimization for different methane feedstock, which will bring enormous advantages for increasing the exploitation of natural gas and biogas.



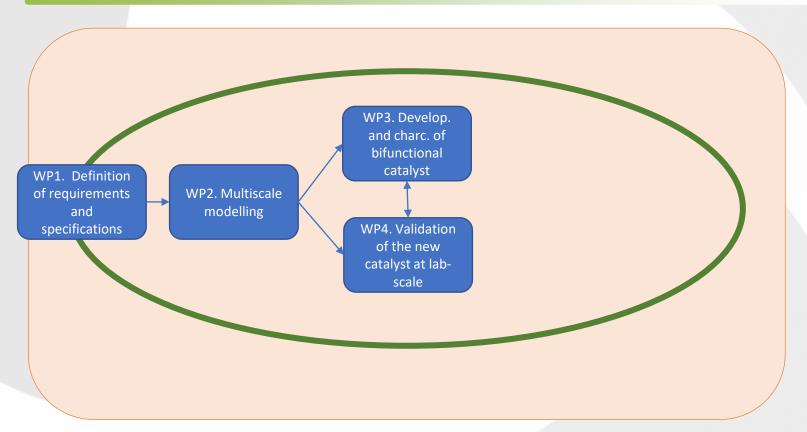




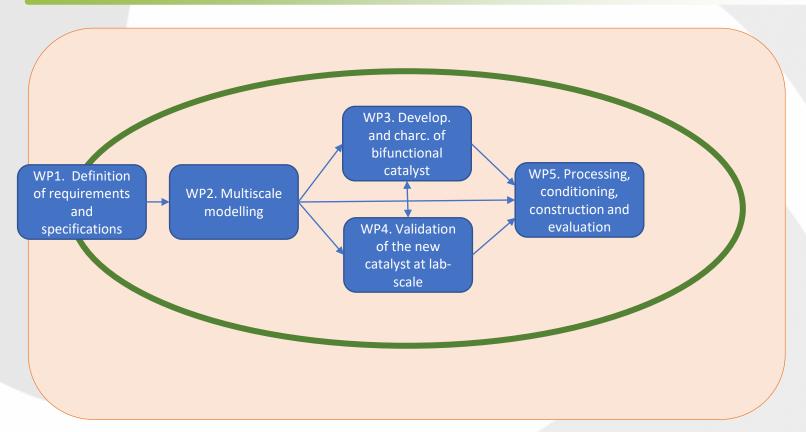




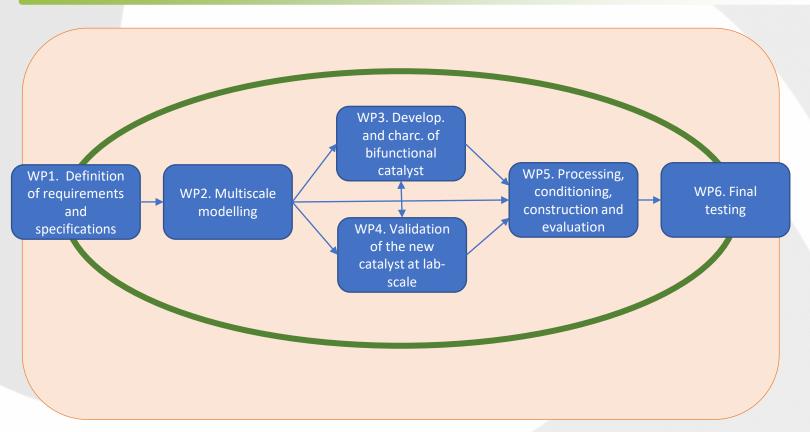




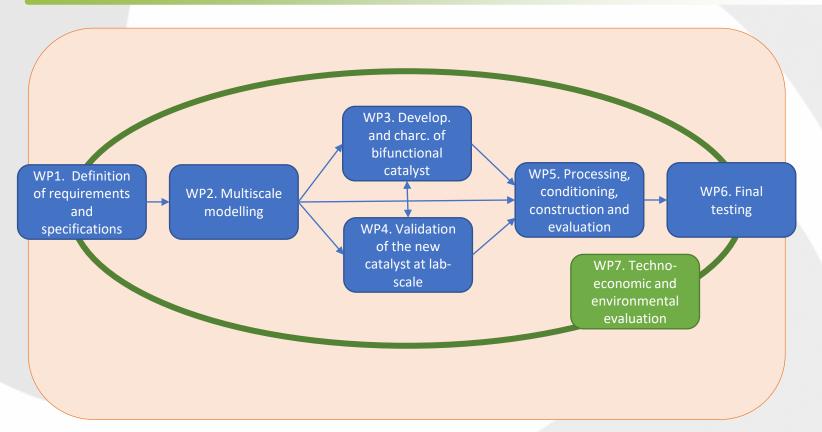




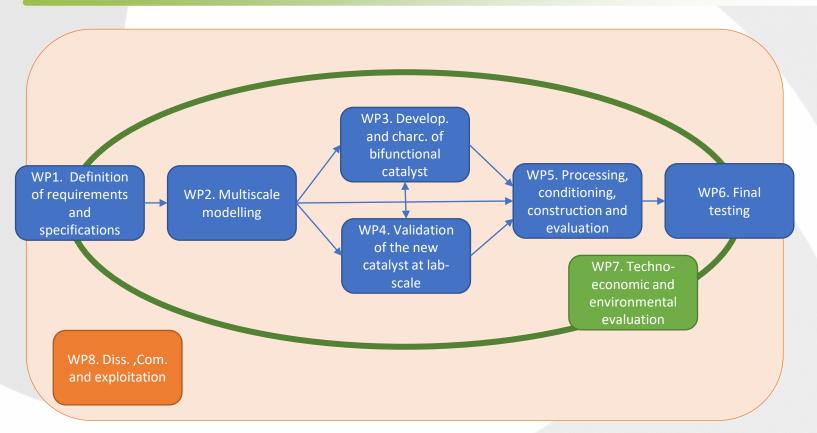




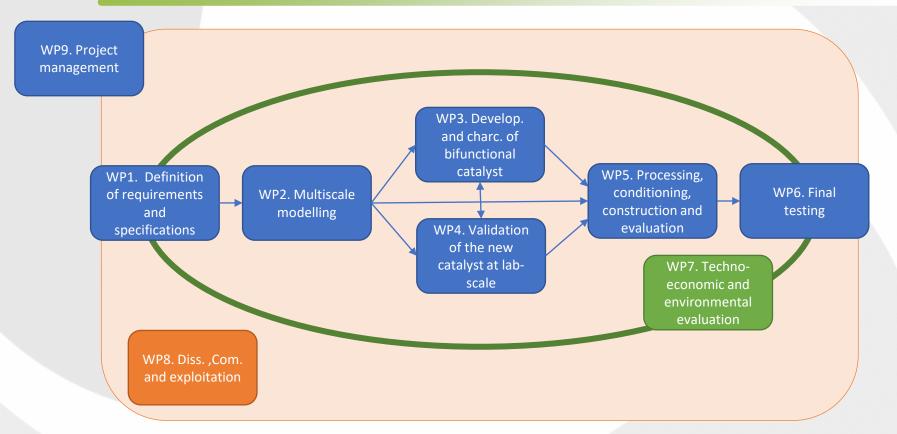














# Partners

### **Partners**









Year 1	Year 2	Year 3	Year 4
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 28 29 30 31 32 33 34 35 36	37 38 39 40 41
WP1 M1-M6			
WP2: Multi-scale modelling M1	-M34		
WP3: Development a	nd characterization of bifunctional catal	yst <b>M5-M33</b>	
	<b>WP4:</b> Validation of new catalyst	at lab-scale M13-M36	
WP5: Processing and o	onditioning M5-M38		
		WP6: Final testing M27-	M40
	WP7: Techno-economic and env	ironmental evaluation and risk assessm	ent <b>M12-M42</b>
WP8: Dissemination, communication	and exploitation M1-M42		
WP9: Project management M1-	M42		
WP10: Ethics requirements	M1-M42		



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24 / 55 Deliverables submitted	(18 accepted by the	t ab-scale M13-M36	
Commission) rocessing and conditi	oning M5-M38		
		WP6: Final testing	M27-M40
First milestone planned for M2	WP7: Techno-economic and envi	ronmental evaluation and risk ass	essment M12-M42
First milestone planned for M26 WP8: Dissemination, communication and ex			
WP9: Project management M1-M42			
WP10: Ethics requirements	M1-M42		

## Thank you



### Any questions?

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